Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2023 – 04:19 pm GMT

PDB ID	:	2BYR
Title	:	CRYSTAL STRUCTURE OF ACHBP FROM APLYSIA CALIFORNICA in complex with methyllycaconitine
Authors	:	Hansen, S.B.; Sulzenbacher, G.; Huxford, T.; Marchot, P.; Taylor, P.; Bourne, Y.
Deposited on	:	2005-08-03
Resolution	:	2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

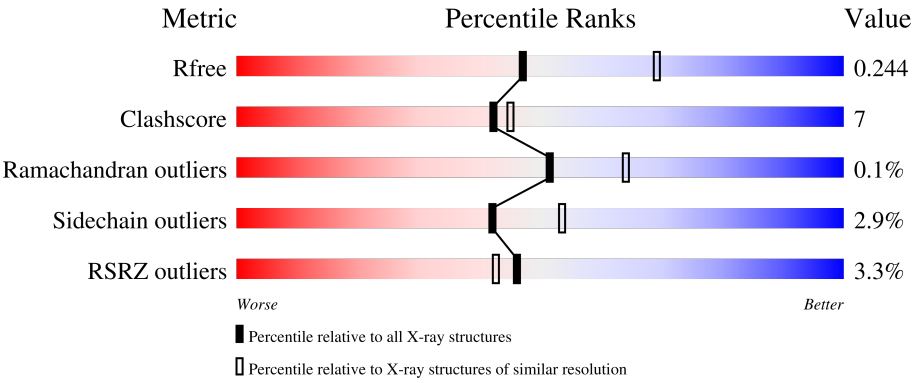
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	227	80% 11% 6%
1	B	227	81% 11% 7%
1	C	227	81% 11% 7%
1	D	227	82% 11% 7%

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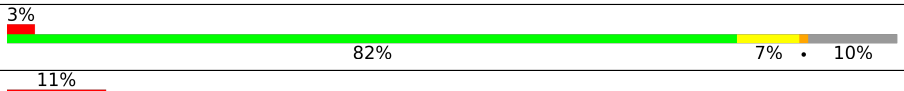
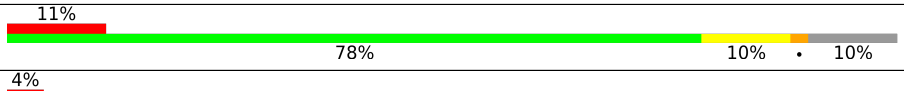
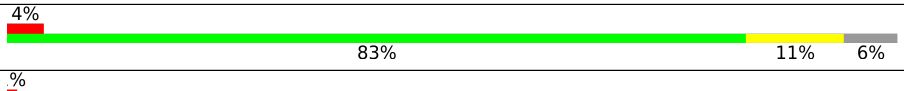
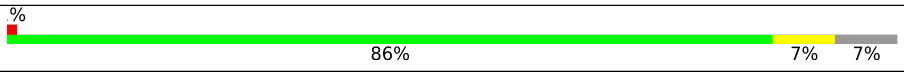
Mol	Chain	Length	Quality of chain
1	E	227	
1	F	227	
1	G	227	
1	H	227	
1	I	227	
1	J	227	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18062 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ACETYLCHOLINE-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	7	0
			1737	1096	289	342	10			
1	B	210	Total	C	N	O	S	0	8	0
			1714	1082	288	334	10			
1	C	210	Total	C	N	O	S	0	5	0
			1699	1073	284	333	9			
1	D	211	Total	C	N	O	S	0	6	0
			1720	1084	290	337	9			
1	E	214	Total	C	N	O	S	0	4	0
			1733	1090	290	343	10			
1	F	209	Total	C	N	O	S	0	6	0
			1700	1074	284	333	9			
1	G	205	Total	C	N	O	S	0	1	0
			1637	1035	267	326	9			
1	H	204	Total	C	N	O	S	0	1	0
			1634	1032	270	324	8			
1	I	213	Total	C	N	O	S	0	4	0
			1724	1085	287	343	9			
1	J	212	Total	C	N	O	S	0	5	0
			1718	1084	285	339	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	TYR	-	expression tag	UNP Q8WSF8
A	-6	LYS	-	expression tag	UNP Q8WSF8
A	-5	ASP	-	expression tag	UNP Q8WSF8
A	-4	ASP	-	expression tag	UNP Q8WSF8
A	-3	ASP	-	expression tag	UNP Q8WSF8
A	-2	ASP	-	expression tag	UNP Q8WSF8
A	-1	LYS	-	expression tag	UNP Q8WSF8
A	0	LEU	-	expression tag	UNP Q8WSF8
B	-7	TYR	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	LYS	-	expression tag	UNP Q8WSF8
B	-5	ASP	-	expression tag	UNP Q8WSF8
B	-4	ASP	-	expression tag	UNP Q8WSF8
B	-3	ASP	-	expression tag	UNP Q8WSF8
B	-2	ASP	-	expression tag	UNP Q8WSF8
B	-1	LYS	-	expression tag	UNP Q8WSF8
B	0	LEU	-	expression tag	UNP Q8WSF8
C	-7	TYR	-	expression tag	UNP Q8WSF8
C	-6	LYS	-	expression tag	UNP Q8WSF8
C	-5	ASP	-	expression tag	UNP Q8WSF8
C	-4	ASP	-	expression tag	UNP Q8WSF8
C	-3	ASP	-	expression tag	UNP Q8WSF8
C	-2	ASP	-	expression tag	UNP Q8WSF8
C	-1	LYS	-	expression tag	UNP Q8WSF8
C	0	LEU	-	expression tag	UNP Q8WSF8
D	-7	TYR	-	expression tag	UNP Q8WSF8
D	-6	LYS	-	expression tag	UNP Q8WSF8
D	-5	ASP	-	expression tag	UNP Q8WSF8
D	-4	ASP	-	expression tag	UNP Q8WSF8
D	-3	ASP	-	expression tag	UNP Q8WSF8
D	-2	ASP	-	expression tag	UNP Q8WSF8
D	-1	LYS	-	expression tag	UNP Q8WSF8
D	0	LEU	-	expression tag	UNP Q8WSF8
E	-7	TYR	-	expression tag	UNP Q8WSF8
E	-6	LYS	-	expression tag	UNP Q8WSF8
E	-5	ASP	-	expression tag	UNP Q8WSF8
E	-4	ASP	-	expression tag	UNP Q8WSF8
E	-3	ASP	-	expression tag	UNP Q8WSF8
E	-2	ASP	-	expression tag	UNP Q8WSF8
E	-1	LYS	-	expression tag	UNP Q8WSF8
E	0	LEU	-	expression tag	UNP Q8WSF8
F	-7	TYR	-	expression tag	UNP Q8WSF8
F	-6	LYS	-	expression tag	UNP Q8WSF8
F	-5	ASP	-	expression tag	UNP Q8WSF8
F	-4	ASP	-	expression tag	UNP Q8WSF8
F	-3	ASP	-	expression tag	UNP Q8WSF8
F	-2	ASP	-	expression tag	UNP Q8WSF8
F	-1	LYS	-	expression tag	UNP Q8WSF8
F	0	LEU	-	expression tag	UNP Q8WSF8
G	-7	TYR	-	expression tag	UNP Q8WSF8
G	-6	LYS	-	expression tag	UNP Q8WSF8
G	-5	ASP	-	expression tag	UNP Q8WSF8

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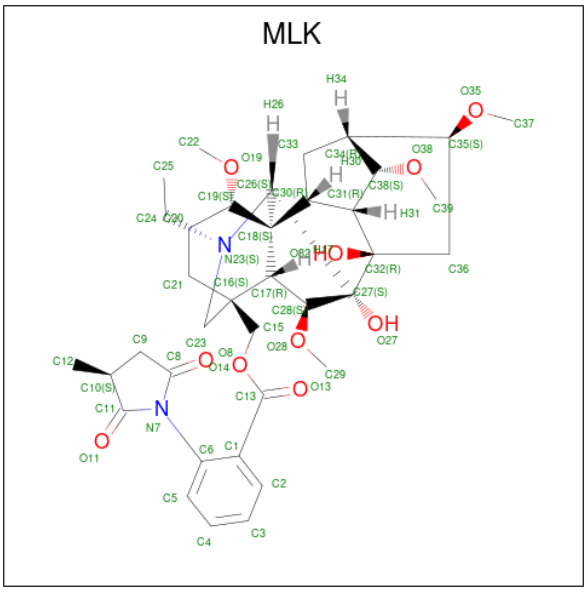
Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	ASP	-	expression tag	UNP Q8WSF8
G	-3	ASP	-	expression tag	UNP Q8WSF8
G	-2	ASP	-	expression tag	UNP Q8WSF8
G	-1	LYS	-	expression tag	UNP Q8WSF8
G	0	LEU	-	expression tag	UNP Q8WSF8
H	-7	TYR	-	expression tag	UNP Q8WSF8
H	-6	LYS	-	expression tag	UNP Q8WSF8
H	-5	ASP	-	expression tag	UNP Q8WSF8
H	-4	ASP	-	expression tag	UNP Q8WSF8
H	-3	ASP	-	expression tag	UNP Q8WSF8
H	-2	ASP	-	expression tag	UNP Q8WSF8
H	-1	LYS	-	expression tag	UNP Q8WSF8
H	0	LEU	-	expression tag	UNP Q8WSF8
I	-7	TYR	-	expression tag	UNP Q8WSF8
I	-6	LYS	-	expression tag	UNP Q8WSF8
I	-5	ASP	-	expression tag	UNP Q8WSF8
I	-4	ASP	-	expression tag	UNP Q8WSF8
I	-3	ASP	-	expression tag	UNP Q8WSF8
I	-2	ASP	-	expression tag	UNP Q8WSF8
I	-1	LYS	-	expression tag	UNP Q8WSF8
I	0	LEU	-	expression tag	UNP Q8WSF8
J	-7	TYR	-	expression tag	UNP Q8WSF8
J	-6	LYS	-	expression tag	UNP Q8WSF8
J	-5	ASP	-	expression tag	UNP Q8WSF8
J	-4	ASP	-	expression tag	UNP Q8WSF8
J	-3	ASP	-	expression tag	UNP Q8WSF8
J	-2	ASP	-	expression tag	UNP Q8WSF8
J	-1	LYS	-	expression tag	UNP Q8WSF8
J	0	LEU	-	expression tag	UNP Q8WSF8

- Molecule 2 is METHYLLYCACONITINE (three-letter code: MLK) (formula: $C_{37}H_{50}N_2O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 49 37 2 10	0	0
2	B	1	Total C N O 49 37 2 10	0	0
2	C	1	Total C N O 49 37 2 10	0	0
2	D	1	Total C N O 49 37 2 10	0	0
2	E	1	Total C N O 49 37 2 10	0	0
2	F	1	Total C N O 49 37 2 10	0	0
2	G	1	Total C N O 49 37 2 10	0	0
2	H	1	Total C N O 49 37 2 10	0	0
2	I	1	Total C N O 49 37 2 10	0	0
2	J	1	Total C N O 49 37 2 10	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	113	Total O 113 113	0	0
3	B	91	Total O 91 91	0	0

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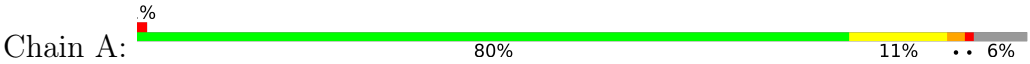
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	54	Total O 54 54	0	0
3	D	58	Total O 58 58	0	0
3	E	88	Total O 88 88	0	0
3	F	32	Total O 32 32	0	0
3	G	23	Total O 23 23	0	0
3	H	14	Total O 14 14	0	0
3	I	29	Total O 29 29	0	0
3	J	54	Total O 54 54	0	0

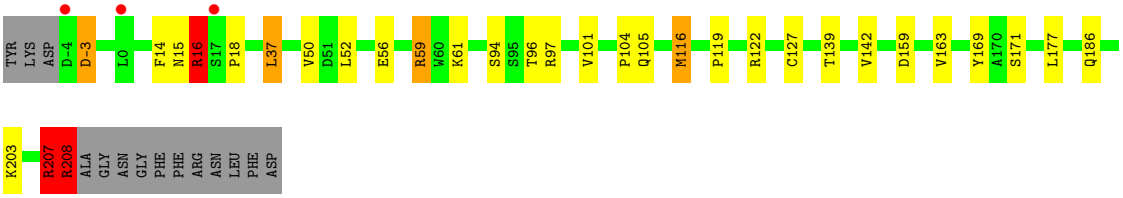
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

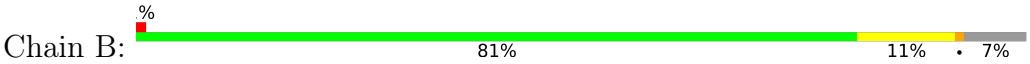
Chain A:

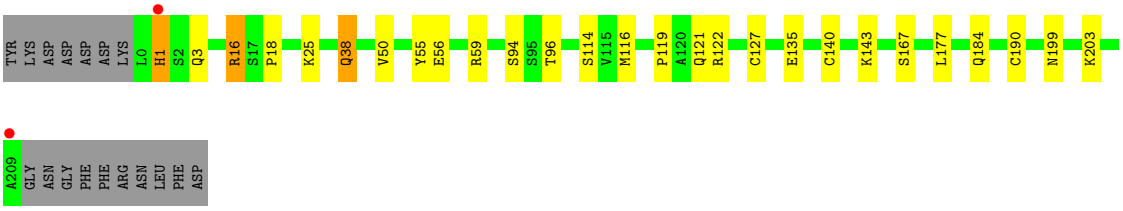




• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

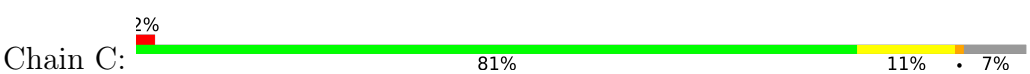
Chain B:

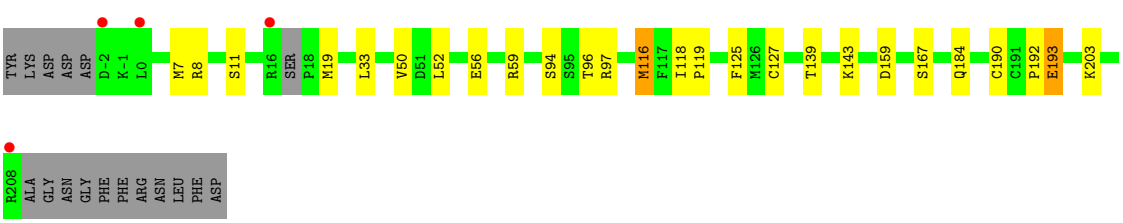




• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

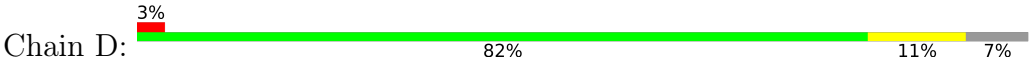
Chain C:

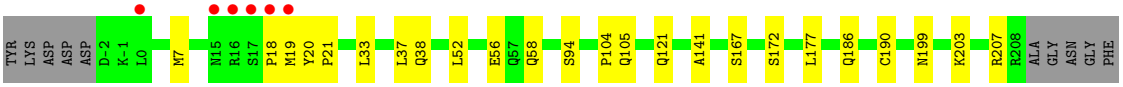




• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

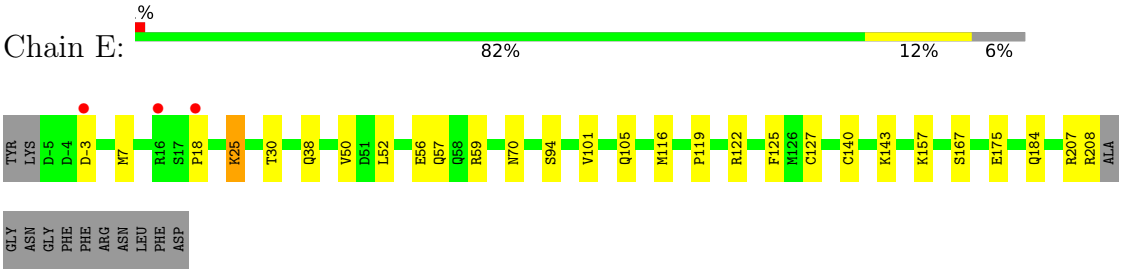
Chain D:





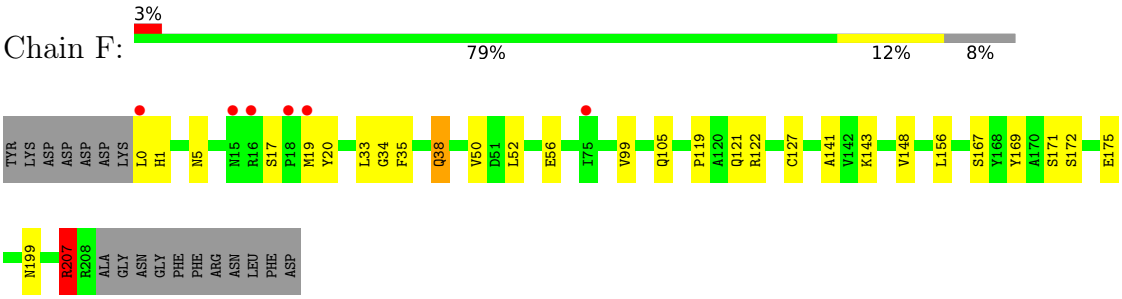
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain E:



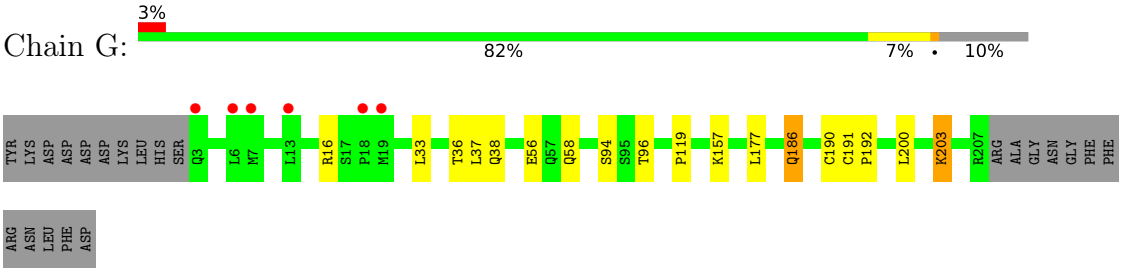
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain F:



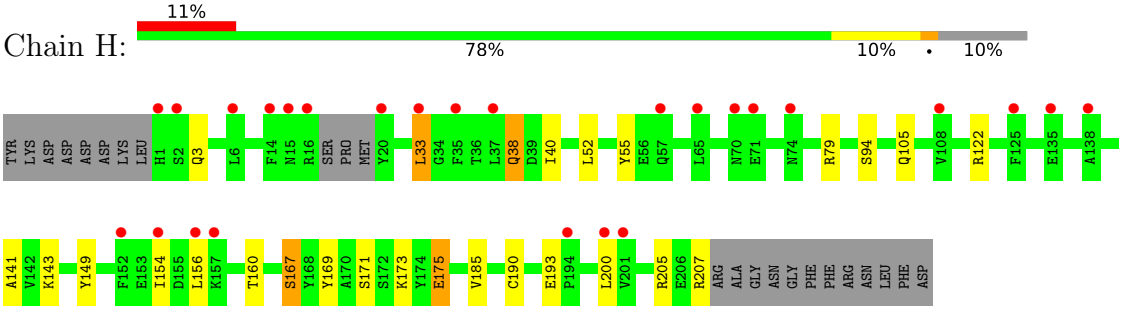
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain G:



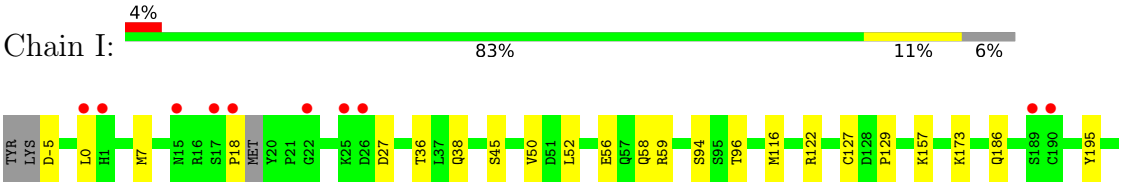
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

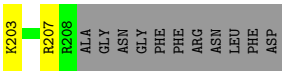
Chain H:



• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain I:





• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.27Å 135.78Å 147.29Å 90.00° 99.46° 90.00°	Depositor
Resolution (Å)	20.00 – 2.45 66.35 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.45) 98.5 (66.35-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.193 , 0.232 0.211 , 0.244	Depositor DCC
R_{free} test set	1891 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18062	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLK

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.48	0/1806	0.71	3/2458 (0.1%)
1	B	0.46	0/1787	0.64	2/2432 (0.1%)
1	C	0.43	0/1761	0.63	0/2397
1	D	0.40	0/1785	0.62	0/2430
1	E	0.46	0/1790	0.63	1/2437 (0.0%)
1	F	0.40	0/1765	0.65	2/2405 (0.1%)
1	G	0.39	0/1681	0.57	0/2293
1	H	0.38	0/1677	0.55	0/2286
1	I	0.39	0/1779	0.57	0/2422
1	J	0.41	0/1779	0.58	0/2422
All	All	0.42	0/17610	0.62	8/23982 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	6

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	208	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	F	207[A]	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	F	207[B]	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	A	16	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	140	CYS	CA-CB-SG	-5.54	104.04	114.00
1	B	16	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	207	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	E	140	CYS	CA-CB-SG	-5.03	104.95	114.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1	HIS	Peptide
1	C	190	CYS	Peptide
1	D	190	CYS	Peptide
1	F	0	LEU	Peptide
1	G	190	CYS	Peptide
1	H	190	CYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1737	0	1672	35	0
1	B	1714	0	1655	27	0
1	C	1699	0	1634	15	0
1	D	1720	0	1656	23	0
1	E	1733	0	1661	23	0
1	F	1700	0	1637	31	0
1	G	1637	0	1565	14	0
1	H	1634	0	1563	16	0
1	I	1724	0	1650	36	0
1	J	1718	0	1652	17	0
2	A	49	0	50	4	0
2	B	49	0	50	3	0
2	C	49	0	50	3	0
2	D	49	0	50	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	49	0	50	7	0
2	F	49	0	50	6	0
2	G	49	0	50	4	0
2	H	49	0	50	6	0
2	I	49	0	50	6	0
2	J	49	0	50	3	0
3	A	113	0	0	1	0
3	B	91	0	0	3	0
3	C	54	0	0	0	0
3	D	58	0	0	1	0
3	E	88	0	0	3	0
3	F	32	0	0	1	0
3	G	23	0	0	0	0
3	H	14	0	0	0	0
3	I	29	0	0	1	0
3	J	54	0	0	0	0
All	All	18062	0	16845	237	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (237) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59[B]:ARG:HD3	1:A:116[B]:MET:CE	1.17	1.60
1:I:59[B]:ARG:CG	1:I:116[B]:MET:HE3	1.31	1.54
1:I:59[B]:ARG:CG	1:I:116[B]:MET:CE	1.94	1.46
1:A:59[B]:ARG:CD	1:A:116[B]:MET:CE	2.09	1.28
1:A:59[B]:ARG:CD	1:A:116[B]:MET:HE2	1.65	1.19
1:I:59[B]:ARG:HG3	1:I:116[B]:MET:CE	1.60	1.19
1:I:59[B]:ARG:CD	1:I:116[B]:MET:HE3	1.88	1.03
1:A:59[B]:ARG:HD3	1:A:116[B]:MET:HE1	1.43	1.01
1:I:59[B]:ARG:CD	1:I:116[B]:MET:CE	2.37	1.00
1:I:59[B]:ARG:HG2	1:I:116[B]:MET:HE3	0.95	0.94
1:G:186:GLN:HE22	2:G:301:MLK:H4	1.34	0.91
1:I:59[B]:ARG:HG3	1:I:116[B]:MET:HE1	1.53	0.91
1:A:59[B]:ARG:HD3	1:A:116[B]:MET:SD	2.14	0.86
1:F:171:SER:HA	1:F:207[B]:ARG:HH12	1.40	0.86
1:A:59[B]:ARG:CD	1:A:116[B]:MET:HE1	2.01	0.86
1:F:207[A]:ARG:HH21	1:F:207[A]:ARG:HG2	1.39	0.86
1:D:37:LEU:HD11	1:D:52:LEU:HD11	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:THR:OG1	1:C:203:LYS:NZ	2.10	0.84
1:I:59[A]:ARG:HH11	1:I:116[A]:MET:CE	1.90	0.84
1:I:59[B]:ARG:CG	1:I:116[B]:MET:HE1	2.03	0.82
1:H:38:GLN:HE21	1:H:38:GLN:HA	1.41	0.82
1:I:59[B]:ARG:HD3	1:I:116[B]:MET:CE	2.12	0.80
1:I:59[B]:ARG:CD	1:I:116[B]:MET:HE1	2.10	0.79
1:A:59[B]:ARG:CG	1:A:116[B]:MET:SD	2.72	0.78
1:A:59[B]:ARG:HD3	1:A:116[B]:MET:HE2	0.78	0.77
1:I:59[B]:ARG:HG2	1:I:116[B]:MET:CE	1.82	0.76
2:F:301:MLK:C12	1:J:38[B]:GLN:HE21	1.99	0.76
1:B:143:LYS:HE3	1:B:184:GLN:HE22	1.51	0.75
1:C:97[B]:ARG:HH11	1:C:97[B]:ARG:HG3	1.53	0.73
1:I:59[A]:ARG:HH11	1:I:116[A]:MET:HE1	1.51	0.73
2:F:301:MLK:H122	1:J:38[B]:GLN:HE21	1.53	0.73
1:H:173:LYS:NZ	1:I:45:SER:O	2.22	0.72
1:A:59[B]:ARG:NE	1:A:116[B]:MET:HE1	2.05	0.71
1:D:207[B]:ARG:HH21	1:D:207[B]:ARG:HG3	1.55	0.71
1:B:59[B]:ARG:HH21	1:B:59[B]:ARG:HG3	1.55	0.70
1:I:59[B]:ARG:HG3	1:I:116[B]:MET:HE2	1.68	0.70
1:G:38[B]:GLN:NE2	2:H:301:MLK:H122	2.06	0.70
1:I:186:GLN:HE22	2:I:301:MLK:C4	2.05	0.69
1:F:171:SER:CA	1:F:207[B]:ARG:HH12	2.06	0.69
1:C:192:PRO:HD2	1:C:193:GLU:OE2	1.93	0.68
1:C:50:VAL:HG21	1:C:127:CYS:SG	2.34	0.68
1:C:52:LEU:HG	1:C:125:PHE:HE2	1.60	0.67
1:B:50:VAL:HG21	1:B:127:CYS:SG	2.36	0.66
1:J:177:LEU:HB2	1:J:203[A]:LYS:HG2	1.77	0.66
1:J:143:LYS:NZ	1:J:184:GLN:HE22	1.94	0.66
1:F:119:PRO:HB2	1:F:121[B]:GLN:HE21	1.62	0.65
1:D:172:SER:O	1:D:207[A]:ARG:HD2	1.95	0.65
1:F:1:HIS:CE1	1:F:5:ASN:HD21	2.14	0.65
1:H:38:GLN:HE22	1:H:167:SER:HB2	1.61	0.65
1:A:59[B]:ARG:CD	1:A:116[B]:MET:SD	2.79	0.64
1:B:25:LYS:NZ	3:B:2004:HOH:O	2.31	0.64
1:E:207[B]:ARG:HG3	1:E:207[B]:ARG:HH11	1.64	0.63
1:A:139:THR:HG23	1:A:203[A]:LYS:HD3	1.79	0.63
1:D:207[B]:ARG:HH21	1:D:207[B]:ARG:CG	2.12	0.63
1:F:38[A]:GLN:HE22	1:F:167:SER:HB3	1.64	0.63
1:A:-3:ASP:OD2	1:A:-3:ASP:C	2.38	0.62
1:D:38[A]:GLN:HE21	2:E:301:MLK:H122	1.65	0.62
1:B:143:LYS:NZ	3:B:2059:HOH:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38[B]:GLN:HE22	2:H:301:MLK:H122	1.63	0.61
2:A:301:MLK:H9C1	1:E:167:SER:HB2	1.82	0.61
1:I:186:GLN:HE22	2:I:301:MLK:H4	1.66	0.60
1:I:59[A]:ARG:HH11	1:I:116[A]:MET:HE2	1.65	0.60
1:F:175:GLU:HB3	1:F:207[B]:ARG:CD	2.31	0.60
1:B:38[A]:GLN:NE2	1:B:167:SER:O	2.35	0.60
1:H:38:GLN:HE21	1:H:38:GLN:CA	2.13	0.60
1:A:16:ARG:HH11	1:A:16:ARG:HG2	1.67	0.59
1:A:16:ARG:HH11	1:A:16:ARG:CG	2.15	0.59
1:G:36:THR:HG22	1:G:38[A]:GLN:HE22	1.67	0.59
1:G:36:THR:HG22	1:G:38[A]:GLN:NE2	2.17	0.59
1:I:59[B]:ARG:HD3	1:I:116[B]:MET:HE3	1.73	0.59
1:I:36:THR:HG22	1:I:38[B]:GLN:HE22	1.66	0.59
1:D:38[A]:GLN:HE21	2:E:301:MLK:C12	2.16	0.58
1:G:186:GLN:HE22	2:G:301:MLK:C4	2.11	0.58
1:E:207[B]:ARG:HH11	1:E:207[B]:ARG:CG	2.17	0.58
1:A:104:PRO:C	1:A:105[B]:GLN:HE21	2.08	0.58
1:D:172:SER:O	1:D:207[A]:ARG:CD	2.52	0.58
1:I:207:ARG:HH21	1:I:207:ARG:HG3	1.69	0.57
1:F:171:SER:HA	1:F:207[B]:ARG:NH1	2.15	0.57
1:H:94:SER:HB3	2:H:301:MLK:H121	1.87	0.56
1:F:119:PRO:HG2	1:F:121[B]:GLN:HE22	1.71	0.56
1:E:143:LYS:HE3	1:E:184:GLN:HE22	1.70	0.56
1:A:59[B]:ARG:HG2	1:A:116[B]:MET:SD	2.46	0.55
1:B:143:LYS:HE3	1:B:184:GLN:NE2	2.21	0.55
1:A:207:ARG:HG2	1:A:207:ARG:HH11	1.71	0.55
1:E:175:GLU:HB3	1:E:207[B]:ARG:NH1	2.21	0.55
1:C:94:SER:HB3	2:C:301:MLK:H121	1.88	0.55
1:J:143:LYS:HZ2	1:J:184:GLN:HE22	1.54	0.55
1:B:59[A]:ARG:HD2	1:B:116[A]:MET:CE	2.37	0.55
1:B:59[B]:ARG:HH21	1:B:59[B]:ARG:CG	2.20	0.55
1:F:169:TYR:CZ	1:F:171:SER:HB2	2.42	0.55
1:B:50:VAL:CG2	1:B:127:CYS:SG	2.95	0.55
1:C:143:LYS:NZ	1:C:184:GLN:HE22	2.05	0.55
1:I:7:MET:SD	1:J:18:PRO:HB2	2.47	0.54
1:J:50:VAL:HG21	1:J:127:CYS:SG	2.47	0.54
2:E:301:MLK:H31	2:E:301:MLK:O28	2.06	0.54
1:G:177:LEU:HB2	1:G:203:LYS:HG2	1.88	0.54
1:D:94:SER:HB3	2:D:301:MLK:H121	1.88	0.54
1:B:122:ARG:HD2	1:C:96:THR:O	2.08	0.53
1:D:56:GLU:OE2	1:D:58:GLN:NE2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:SER:HB2	2:E:301:MLK:H9C1	1.90	0.53
1:A:18:PRO:HB2	1:E:7:MET:SD	2.48	0.53
1:B:16:ARG:HG3	1:B:16:ARG:HH11	1.74	0.52
1:A:208:ARG:HH11	1:A:208:ARG:CG	2.22	0.52
1:D:37:LEU:HD11	1:D:52:LEU:CD1	2.35	0.52
1:E:57:GLN:NE2	3:E:2022:HOH:O	2.29	0.52
1:F:50:VAL:HG21	1:F:127:CYS:SG	2.51	0.51
1:E:50:VAL:HG21	1:E:127:CYS:SG	2.51	0.50
1:F:119:PRO:HB2	1:F:121[B]:GLN:NE2	2.25	0.50
1:I:38[A]:GLN:HE21	2:J:301:MLK:H122	1.77	0.50
2:B:301:MLK:H31	2:B:301:MLK:O28	2.10	0.50
1:E:175:GLU:HB3	1:E:207[B]:ARG:HH12	1.76	0.50
1:D:141:ALA:HB1	1:D:199:ASN:HD21	1.76	0.50
1:D:56:GLU:CD	1:D:58:GLN:HE21	2.14	0.49
1:B:177:LEU:HD12	1:B:203[B]:LYS:HG2	1.95	0.49
1:G:94:SER:HB3	2:G:301:MLK:H121	1.94	0.49
2:F:301:MLK:H123	1:J:38[B]:GLN:HE21	1.75	0.49
1:H:122:ARG:HD2	1:I:96:THR:O	2.12	0.49
1:F:141:ALA:HB1	1:F:199:ASN:HD21	1.78	0.49
2:I:301:MLK:H31	2:I:301:MLK:O28	2.12	0.49
1:A:50:VAL:HG21	1:A:127:CYS:SG	2.53	0.49
2:J:301:MLK:H31	2:J:301:MLK:O28	2.13	0.48
1:E:56:GLU:O	1:E:119:PRO:HD2	2.14	0.48
1:C:167:SER:HB2	2:D:301:MLK:H9C1	1.94	0.48
1:F:171:SER:C	1:F:207[B]:ARG:HH12	2.17	0.48
2:F:301:MLK:O28	2:F:301:MLK:H31	2.14	0.48
1:D:104:PRO:C	1:D:105[B]:GLN:HE21	2.17	0.48
1:A:59[B]:ARG:HG3	1:A:116[B]:MET:SD	2.53	0.48
1:C:56:GLU:O	1:C:119:PRO:HD2	2.13	0.48
1:A:37:LEU:HD13	1:A:163:VAL:HG11	1.95	0.48
1:A:122:ARG:HD2	1:B:96:THR:O	2.14	0.48
1:D:177:LEU:HD12	1:D:203:LYS:HG2	1.96	0.48
1:E:59[A]:ARG:HG2	1:E:116[A]:MET:SD	2.53	0.48
2:G:301:MLK:H31	2:G:301:MLK:O28	2.13	0.48
1:I:186:GLN:NE2	2:I:301:MLK:H4	2.29	0.48
1:C:50:VAL:CG2	1:C:127:CYS:SG	3.01	0.48
1:H:3:GLN:NE2	1:I:27:ASP:OD2	2.41	0.48
2:A:301:MLK:C9	1:E:167:SER:HB2	2.43	0.47
1:F:105[B]:GLN:OE1	1:F:119:PRO:HB3	2.14	0.47
1:H:38:GLN:HA	1:H:38:GLN:NE2	2.19	0.47
1:J:38[A]:GLN:NE2	1:J:167:SER:OG	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:SER:HB2	2:C:301:MLK:H9C1	1.96	0.47
3:F:2002:HOH:O	1:J:3:GLN:HG2	2.13	0.47
1:E:30:THR:CG2	1:E:157:LYS:HG3	2.45	0.47
1:E:38:GLN:HE21	1:E:38:GLN:HA	1.80	0.47
2:A:301:MLK:O28	2:A:301:MLK:H31	2.15	0.47
1:H:38:GLN:OE1	1:H:55:TYR:CE1	2.68	0.47
1:E:59[A]:ARG:HD3	1:E:116[A]:MET:HE1	1.96	0.47
1:H:175:GLU:HB3	1:H:207:ARG:HG3	1.96	0.47
1:E:52:LEU:HG	1:E:125:PHE:HE2	1.80	0.46
1:A:94:SER:HB3	2:A:301:MLK:H121	1.96	0.46
1:I:59[B]:ARG:NE	1:I:116[B]:MET:HE1	2.30	0.46
1:D:7:MET:SD	1:E:18:PRO:HB2	2.55	0.46
1:E:59[A]:ARG:HD3	1:E:116[A]:MET:CE	2.46	0.46
1:G:56:GLU:OE2	1:G:58:GLN:NE2	2.38	0.46
1:A:207:ARG:HD3	3:A:2095:HOH:O	2.15	0.46
1:B:59[B]:ARG:CZ	1:B:114[B]:SER:HB2	2.46	0.46
1:F:119:PRO:HG2	1:F:121[B]:GLN:NE2	2.30	0.46
1:B:94:SER:HB3	2:B:301:MLK:H121	1.99	0.45
1:A:96:THR:O	1:E:122:ARG:HD2	2.16	0.45
1:A:177:LEU:HB2	1:A:203[B]:LYS:HG2	1.98	0.45
1:G:37:LEU:C	1:G:38[A]:GLN:HE21	2.20	0.45
1:C:116:MET:SD	1:C:118:ILE:HD11	2.57	0.45
1:I:195:TYR:HE1	2:I:301:MLK:H222	1.82	0.45
1:C:97[B]:ARG:HH11	1:C:97[B]:ARG:CG	2.27	0.45
1:E:38:GLN:HA	1:E:38:GLN:NE2	2.31	0.45
1:E:25:LYS:NZ	3:E:2004:HOH:O	2.46	0.44
1:F:19:MET:HG3	1:F:20:TYR:N	2.32	0.44
1:A:59[A]:ARG:NH2	1:A:61:LYS:HB2	2.31	0.44
1:A:139:THR:OG1	1:A:203[A]:LYS:HD2	2.18	0.44
1:H:149:TYR:CD2	1:H:154:ILE:HD12	2.52	0.44
1:I:122:ARG:HD2	1:J:96:THR:O	2.18	0.44
1:G:38[B]:GLN:CD	2:H:301:MLK:H122	2.37	0.44
1:G:56:GLU:O	1:G:119:PRO:HD2	2.18	0.44
1:J:50:VAL:CG2	1:J:127:CYS:SG	3.06	0.44
1:B:16:ARG:HH11	1:B:16:ARG:CG	2.30	0.44
1:F:33[A]:LEU:HD21	1:F:35:PHE:CZ	2.52	0.44
1:F:33[A]:LEU:HD23	1:F:34:GLY:N	2.33	0.43
1:I:56:GLU:OE2	1:I:58:GLN:NE2	2.43	0.43
1:I:59[A]:ARG:HE	1:I:116[A]:MET:HE2	1.83	0.43
2:H:301:MLK:O28	2:H:301:MLK:H31	2.19	0.43
1:B:199:ASN:ND2	3:B:2059:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:ARG:HD2	1:G:96:THR:O	2.19	0.43
1:F:207[A]:ARG:HG2	1:F:207[A]:ARG:NH2	2.14	0.43
1:H:33:LEU:HD12	1:H:156:LEU:HD22	1.99	0.43
1:F:56:GLU:O	1:F:119:PRO:HD2	2.19	0.43
1:A:169:TYR:CZ	1:A:171:SER:HB2	2.54	0.43
1:I:59[A]:ARG:NH1	1:I:116[A]:MET:HE1	2.27	0.43
1:H:141:ALA:HA	1:H:200:LEU:O	2.18	0.43
1:H:40:ILE:HG12	1:H:52:LEU:HD22	2.01	0.42
1:A:14:PHE:C	1:A:15:ASN:HD22	2.23	0.42
1:F:143:LYS:HD2	2:F:301:MLK:C5	2.49	0.42
1:C:7:MET:HG2	3:D:2003:HOH:O	2.20	0.42
1:B:190:CYS:SG	2:B:301:MLK:H393	2.59	0.42
2:E:301:MLK:O28	2:E:301:MLK:C31	2.68	0.42
1:I:173:LYS:HE3	1:J:45:SER:O	2.19	0.42
1:A:56:GLU:O	1:A:119:PRO:HD2	2.20	0.42
1:B:38[B]:GLN:OE1	1:B:55:TYR:CE2	2.73	0.42
1:B:1:HIS:C	1:B:3:GLN:N	2.73	0.41
1:B:56:GLU:O	1:B:119:PRO:HD2	2.20	0.41
1:F:172:SER:O	1:F:207[B]:ARG:CZ	2.68	0.41
1:H:143:LYS:HD2	2:H:301:MLK:O11	2.19	0.41
1:H:169:TYR:CZ	1:H:171:SER:HB2	2.55	0.41
1:J:143:LYS:HZ1	1:J:184:GLN:HE22	1.66	0.41
1:I:18:PRO:C	3:I:2003:HOH:O	2.58	0.41
2:E:301:MLK:H242	2:E:301:MLK:O27	2.19	0.41
1:B:59[B]:ARG:CG	1:B:59[B]:ARG:NH2	2.82	0.41
1:E:94:SER:HB3	2:E:301:MLK:H121	2.03	0.41
1:F:175:GLU:HB3	1:F:207[B]:ARG:HD3	1.99	0.41
1:D:56:GLU:HB3	1:D:121[B]:GLN:HE22	1.85	0.41
2:F:301:MLK:H9C1	1:J:167:SER:HB2	2.02	0.41
1:I:127:CYS:O	1:I:129:PRO:HD3	2.20	0.41
2:I:301:MLK:O27	2:I:301:MLK:H242	2.20	0.41
1:G:191:CYS:HA	1:G:192:PRO:HD3	1.95	0.41
1:C:59[A]:ARG:NH1	1:C:159:ASP:OD1	2.53	0.41
2:C:301:MLK:H31	2:C:301:MLK:O28	2.21	0.41
1:F:99:VAL:HG13	1:F:121[A]:GLN:HB3	2.02	0.41
1:J:195:TYR:CE1	2:J:301:MLK:H222	2.55	0.41
1:D:20:TYR:HA	1:D:21:PRO:HD3	1.95	0.41
1:F:148:VAL:HG21	1:J:106:ILE:HG21	2.02	0.41
1:D:37:LEU:HD12	1:D:37:LEU:HA	1.94	0.40
1:A:59[B]:ARG:NH1	1:A:159:ASP:OD1	2.55	0.40
1:A:97[A]:ARG:HD3	3:E:2045:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:301:MLK:H31	2:D:301:MLK:O28	2.21	0.40
1:E:101:VAL:HG11	1:E:105:GLN:NE2	2.36	0.40
1:I:50:VAL:HG21	1:I:127:CYS:SG	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/227 (96%)	213 (98%)	5 (2%)	0	100	100
1	B	216/227 (95%)	211 (98%)	4 (2%)	1 (0%)	29	34
1	C	211/227 (93%)	206 (98%)	5 (2%)	0	100	100
1	D	215/227 (95%)	209 (97%)	4 (2%)	2 (1%)	17	19
1	E	216/227 (95%)	211 (98%)	5 (2%)	0	100	100
1	F	213/227 (94%)	206 (97%)	7 (3%)	0	100	100
1	G	204/227 (90%)	201 (98%)	3 (2%)	0	100	100
1	H	201/227 (88%)	194 (96%)	7 (4%)	0	100	100
1	I	213/227 (94%)	206 (97%)	7 (3%)	0	100	100
1	J	215/227 (95%)	211 (98%)	4 (2%)	0	100	100
All	All	2122/2270 (94%)	2068 (98%)	51 (2%)	3 (0%)	51	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	18	PRO
1	D	19	MET
1	D	18	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/205 (98%)	188 (94%)	13 (6%)	17	21
1	B	198/205 (97%)	193 (98%)	5 (2%)	47	60
1	C	195/205 (95%)	188 (96%)	7 (4%)	35	46
1	D	198/205 (97%)	196 (99%)	2 (1%)	76	84
1	E	199/205 (97%)	195 (98%)	4 (2%)	55	67
1	F	196/205 (96%)	189 (96%)	7 (4%)	35	46
1	G	187/205 (91%)	181 (97%)	6 (3%)	39	50
1	H	186/205 (91%)	176 (95%)	10 (5%)	22	28
1	I	198/205 (97%)	192 (97%)	6 (3%)	41	52
1	J	198/205 (97%)	195 (98%)	3 (2%)	65	76
All	All	1956/2050 (95%)	1893 (97%)	63 (3%)	42	50

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	ASP
1	A	16	ARG
1	A	37	LEU
1	A	52	LEU
1	A	59[A]	ARG
1	A	59[B]	ARG
1	A	101	VAL
1	A	116[A]	MET
1	A	116[B]	MET
1	A	142	VAL
1	A	186	GLN
1	A	207	ARG
1	A	208	ARG
1	B	38[A]	GLN
1	B	38[B]	GLN
1	B	121[A]	GLN

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Mol	Chain	Res	Type
1	B	121[B]	GLN
1	B	135	GLU
1	C	8	ARG
1	C	11	SER
1	C	19	MET
1	C	33[A]	LEU
1	C	33[B]	LEU
1	C	116	MET
1	C	193	GLU
1	D	33	LEU
1	D	186	GLN
1	E	-3	ASP
1	E	25	LYS
1	E	70	ASN
1	E	208	ARG
1	F	17	SER
1	F	38[A]	GLN
1	F	38[B]	GLN
1	F	52	LEU
1	F	156	LEU
1	F	207[A]	ARG
1	F	207[B]	ARG
1	G	16	ARG
1	G	33	LEU
1	G	157	LYS
1	G	186	GLN
1	G	200	LEU
1	G	203	LYS
1	H	33	LEU
1	H	38	GLN
1	H	79	ARG
1	H	105	GLN
1	H	160	THR
1	H	167	SER
1	H	175	GLU
1	H	185	VAL
1	H	193	GLU
1	H	205	ARG
1	I	-5	ASP
1	I	0	LEU
1	I	52	LEU
1	I	94	SER

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Mol	Chain	Res	Type
1	I	157	LYS
1	I	203	LYS
1	J	17	SER
1	J	19	MET
1	J	207	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	15	ASN
1	A	70	ASN
1	A	199	ASN
1	B	63	ASN
1	B	105	GLN
1	B	184	GLN
1	B	199	ASN
1	C	38	GLN
1	C	74	ASN
1	C	184	GLN
1	D	186	GLN
1	D	199	ASN
1	E	38	GLN
1	E	105	GLN
1	E	184	GLN
1	F	5	ASN
1	F	199	ASN
1	G	15	ASN
1	G	105	GLN
1	G	111	HIS
1	G	186	GLN
1	H	38	GLN
1	H	121	GLN
1	H	162	GLN
1	H	184	GLN
1	I	184	GLN
1	I	186	GLN
1	J	184	GLN
1	J	199	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MLK	E	301	-	54,56,56	1.50	8 (14%)	78,92,92	1.29	10 (12%)
2	MLK	C	301	-	54,56,56	1.56	7 (12%)	78,92,92	1.21	9 (11%)
2	MLK	B	301	-	54,56,56	1.64	7 (12%)	78,92,92	1.17	7 (8%)
2	MLK	D	301	-	54,56,56	1.58	6 (11%)	78,92,92	1.34	11 (14%)
2	MLK	A	301	-	54,56,56	1.49	7 (12%)	78,92,92	1.34	9 (11%)
2	MLK	G	301	-	54,56,56	1.55	7 (12%)	78,92,92	1.18	10 (12%)
2	MLK	H	301	-	54,56,56	1.44	6 (11%)	78,92,92	1.42	10 (12%)
2	MLK	I	301	-	54,56,56	1.52	6 (11%)	78,92,92	1.22	7 (8%)
2	MLK	J	301	-	54,56,56	1.45	7 (12%)	78,92,92	1.36	9 (11%)
2	MLK	F	301	-	54,56,56	1.59	7 (12%)	78,92,92	1.08	8 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLK	E	301	-	-	0/24/141/141	0/2/8/8
2	MLK	C	301	-	-	0/24/141/141	0/2/8/8
2	MLK	B	301	-	-	0/24/141/141	0/2/8/8
2	MLK	D	301	-	-	0/24/141/141	0/2/8/8
2	MLK	A	301	-	-	0/24/141/141	0/2/8/8
2	MLK	G	301	-	-	0/24/141/141	0/2/8/8
2	MLK	H	301	-	-	0/24/141/141	0/2/8/8
2	MLK	I	301	-	-	0/24/141/141	0/2/8/8
2	MLK	J	301	-	-	0/24/141/141	0/2/8/8
2	MLK	F	301	-	-	2/24/141/141	0/2/8/8

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	MLK	C11-N7	-5.80	1.32	1.40
2	I	301	MLK	C1-C6	5.64	1.49	1.41
2	F	301	MLK	C11-N7	-5.48	1.32	1.40
2	E	301	MLK	C1-C6	5.45	1.49	1.41
2	D	301	MLK	C1-C6	5.39	1.49	1.41
2	C	301	MLK	C1-C6	5.29	1.49	1.41
2	H	301	MLK	C1-C6	5.11	1.48	1.41
2	G	301	MLK	C1-C6	5.09	1.48	1.41
2	D	301	MLK	C11-N7	-5.03	1.33	1.40
2	J	301	MLK	C1-C6	5.02	1.48	1.41
2	F	301	MLK	C8-N7	-5.00	1.33	1.40
2	C	301	MLK	C11-N7	-4.98	1.33	1.40
2	F	301	MLK	C1-C6	4.94	1.48	1.41
2	C	301	MLK	C8-N7	-4.92	1.33	1.40
2	D	301	MLK	C8-N7	-4.87	1.33	1.40
2	B	301	MLK	C1-C6	4.79	1.48	1.41
2	G	301	MLK	C8-N7	-4.78	1.33	1.40
2	A	301	MLK	C1-C6	4.76	1.48	1.41
2	B	301	MLK	C8-N7	-4.75	1.33	1.40
2	D	301	MLK	O14-C13	4.73	1.45	1.33
2	A	301	MLK	C11-N7	-4.68	1.33	1.40
2	I	301	MLK	O14-C13	4.67	1.45	1.33
2	H	301	MLK	O14-C13	4.66	1.45	1.33
2	I	301	MLK	C11-N7	-4.63	1.33	1.40
2	E	301	MLK	C11-N7	-4.62	1.33	1.40
2	J	301	MLK	C11-N7	-4.53	1.33	1.40
2	G	301	MLK	O14-C13	4.51	1.44	1.33
2	A	301	MLK	O14-C13	4.45	1.44	1.33
2	H	301	MLK	C8-N7	-4.31	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	301	MLK	C8-N7	-4.28	1.34	1.40
2	G	301	MLK	C11-N7	-4.28	1.34	1.40
2	F	301	MLK	O14-C13	4.22	1.44	1.33
2	J	301	MLK	O14-C13	4.15	1.44	1.33
2	C	301	MLK	O14-C13	4.14	1.44	1.33
2	A	301	MLK	C8-N7	-4.11	1.34	1.40
2	H	301	MLK	C11-N7	-4.05	1.34	1.40
2	E	301	MLK	C8-N7	-3.97	1.34	1.40
2	B	301	MLK	O14-C13	3.95	1.43	1.33
2	E	301	MLK	O14-C13	3.93	1.43	1.33
2	J	301	MLK	C8-N7	-3.81	1.35	1.40
2	B	301	MLK	C6-N7	-3.65	1.39	1.44
2	G	301	MLK	C6-N7	-3.29	1.40	1.44
2	C	301	MLK	C6-N7	-3.27	1.40	1.44
2	F	301	MLK	C6-N7	-3.19	1.40	1.44
2	D	301	MLK	C6-N7	-3.03	1.40	1.44
2	A	301	MLK	C6-N7	-3.01	1.40	1.44
2	G	301	MLK	C32-C27	-2.87	1.53	1.56
2	B	301	MLK	C32-C27	-2.75	1.53	1.56
2	A	301	MLK	C32-C27	-2.74	1.53	1.56
2	E	301	MLK	C6-N7	-2.61	1.41	1.44
2	B	301	MLK	C18-C17	-2.49	1.53	1.56
2	C	301	MLK	C32-C27	-2.47	1.53	1.56
2	J	301	MLK	C32-C27	-2.43	1.53	1.56
2	J	301	MLK	C6-N7	-2.39	1.41	1.44
2	I	301	MLK	C6-N7	-2.35	1.41	1.44
2	D	301	MLK	C18-C17	-2.33	1.53	1.56
2	E	301	MLK	C18-C17	-2.33	1.53	1.56
2	I	301	MLK	C32-C27	-2.26	1.54	1.56
2	H	301	MLK	C6-N7	-2.25	1.41	1.44
2	G	301	MLK	C18-C17	-2.23	1.53	1.56
2	F	301	MLK	C18-C17	-2.21	1.53	1.56
2	C	301	MLK	C18-C17	-2.16	1.53	1.56
2	F	301	MLK	C26-N23	2.16	1.51	1.47
2	E	301	MLK	C32-C27	-2.11	1.54	1.56
2	A	301	MLK	C18-C17	-2.08	1.53	1.56
2	J	301	MLK	C18-C17	-2.07	1.53	1.56
2	H	301	MLK	C18-C17	-2.06	1.53	1.56
2	E	301	MLK	O14-C15	-2.02	1.41	1.45

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	301	MLK	O8-C8-N7	4.62	128.14	124.01
2	H	301	MLK	O8-C8-N7	4.42	127.96	124.01
2	E	301	MLK	O8-C8-N7	4.40	127.94	124.01
2	D	301	MLK	O8-C8-N7	4.37	127.92	124.01
2	I	301	MLK	C10-C11-N7	4.26	110.94	108.26
2	H	301	MLK	C10-C11-N7	4.26	110.94	108.26
2	J	301	MLK	C21-C16-C23	-4.19	107.47	111.43
2	H	301	MLK	C21-C16-C23	-4.11	107.54	111.43
2	A	301	MLK	C21-C16-C23	-3.89	107.75	111.43
2	A	301	MLK	O8-C8-N7	3.85	127.45	124.01
2	A	301	MLK	C10-C11-N7	3.61	110.53	108.26
2	J	301	MLK	O8-C8-C9	-3.51	122.12	127.24
2	H	301	MLK	C6-N7-C8	3.50	126.72	122.67
2	H	301	MLK	O11-C11-N7	3.49	127.71	124.30
2	C	301	MLK	C21-C16-C23	-3.22	108.38	111.43
2	E	301	MLK	C10-C11-N7	3.21	110.28	108.26
2	C	301	MLK	C10-C11-N7	3.21	110.28	108.26
2	E	301	MLK	O8-C8-C9	-3.18	122.61	127.24
2	B	301	MLK	O8-C8-N7	3.12	126.80	124.01
2	A	301	MLK	O14-C13-C1	3.11	118.35	112.21
2	H	301	MLK	O8-C8-C9	-3.09	122.74	127.24
2	I	301	MLK	O14-C13-C1	3.09	118.31	112.21
2	C	301	MLK	C15-O14-C13	3.08	122.78	116.57
2	H	301	MLK	C15-O14-C13	3.07	122.77	116.57
2	D	301	MLK	O14-C13-C1	3.06	118.27	112.21
2	G	301	MLK	O8-C8-N7	3.04	126.73	124.01
2	C	301	MLK	O8-C8-N7	3.00	126.69	124.01
2	D	301	MLK	C21-C16-C23	-2.97	108.62	111.43
2	D	301	MLK	C15-O14-C13	2.96	122.54	116.57
2	D	301	MLK	C10-C11-N7	2.96	110.12	108.26
2	G	301	MLK	O11-C11-N7	2.90	127.13	124.30
2	I	301	MLK	O8-C8-N7	2.89	126.59	124.01
2	J	301	MLK	C10-C11-N7	2.85	110.05	108.26
2	J	301	MLK	C6-N7-C8	2.85	125.96	122.67
2	G	301	MLK	C15-O14-C13	2.85	122.31	116.57
2	C	301	MLK	O14-C13-C1	2.82	117.78	112.21
2	B	301	MLK	O8-C8-C9	-2.79	123.18	127.24
2	E	301	MLK	C6-N7-C8	2.77	125.87	122.67
2	A	301	MLK	O8-C8-C9	-2.74	123.24	127.24
2	D	301	MLK	O8-C8-C9	-2.74	123.25	127.24
2	B	301	MLK	C10-C11-N7	2.70	109.96	108.26
2	I	301	MLK	O8-C8-C9	-2.68	123.33	127.24
2	A	301	MLK	C21-C16-C17	2.68	113.28	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301	MLK	O11-C11-N7	2.67	126.91	124.30
2	A	301	MLK	O11-C11-N7	2.59	126.83	124.30
2	E	301	MLK	C21-C16-C23	-2.56	109.01	111.43
2	D	301	MLK	O38-C38-C31	2.52	119.39	112.42
2	A	301	MLK	C15-O14-C13	2.52	121.65	116.57
2	F	301	MLK	O14-C13-C1	2.50	117.16	112.21
2	I	301	MLK	C21-C16-C23	-2.50	109.07	111.43
2	B	301	MLK	C6-N7-C8	2.50	125.56	122.67
2	G	301	MLK	O14-C13-C1	2.47	117.09	112.21
2	E	301	MLK	O14-C13-C1	2.44	117.03	112.21
2	E	301	MLK	C23-C16-C17	2.43	110.15	108.20
2	G	301	MLK	O8-C8-C9	-2.43	123.71	127.24
2	J	301	MLK	O14-C13-C1	2.41	116.98	112.21
2	H	301	MLK	C6-N7-C11	-2.41	120.42	123.18
2	I	301	MLK	C9-C8-N7	2.39	110.07	108.06
2	F	301	MLK	O8-C8-N7	2.38	126.14	124.01
2	J	301	MLK	O11-C11-N7	2.35	126.59	124.30
2	F	301	MLK	C23-C16-C17	2.34	110.08	108.20
2	B	301	MLK	C9-C8-N7	2.34	110.02	108.06
2	H	301	MLK	O14-C13-C1	2.34	116.83	112.21
2	D	301	MLK	O11-C11-N7	2.33	126.57	124.30
2	F	301	MLK	O11-C11-N7	2.30	126.55	124.30
2	J	301	MLK	C21-C16-C17	2.29	112.80	110.00
2	F	301	MLK	C10-C11-N7	2.28	109.70	108.26
2	H	301	MLK	C21-C16-C17	2.28	112.79	110.00
2	C	301	MLK	O11-C11-N7	2.27	126.52	124.30
2	B	301	MLK	C21-C16-C23	-2.27	109.28	111.43
2	D	301	MLK	C18-C30-C31	2.26	119.73	117.22
2	G	301	MLK	C21-C16-C17	2.25	112.75	110.00
2	J	301	MLK	C23-C16-C17	2.22	109.98	108.20
2	C	301	MLK	O14-C13-O13	-2.16	119.28	123.67
2	F	301	MLK	O14-C13-O13	-2.15	119.31	123.67
2	D	301	MLK	O14-C13-O13	-2.15	119.32	123.67
2	G	301	MLK	C23-C16-C15	2.14	111.20	108.00
2	I	301	MLK	C15-O14-C13	2.13	120.86	116.57
2	G	301	MLK	C10-C11-N7	2.12	109.59	108.26
2	F	301	MLK	O8-C8-C9	-2.12	124.16	127.24
2	C	301	MLK	O8-C8-C9	-2.12	124.16	127.24
2	D	301	MLK	C32-C31-C38	2.10	113.33	111.61
2	E	301	MLK	C23-N23-C24	-2.07	108.26	111.33
2	E	301	MLK	C15-O14-C13	2.07	120.75	116.57
2	G	301	MLK	O19-C19-C18	2.07	112.17	108.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	MLK	O19-C19-C18	2.05	112.14	108.35
2	C	301	MLK	C21-C16-C17	2.05	112.50	110.00
2	A	301	MLK	O14-C13-O13	-2.04	119.53	123.67
2	G	301	MLK	C21-C16-C23	-2.02	109.52	111.43
2	B	301	MLK	C21-C16-C17	2.01	112.46	110.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	301	MLK	O13-C13-O14-C15
2	F	301	MLK	C1-C13-O14-C15

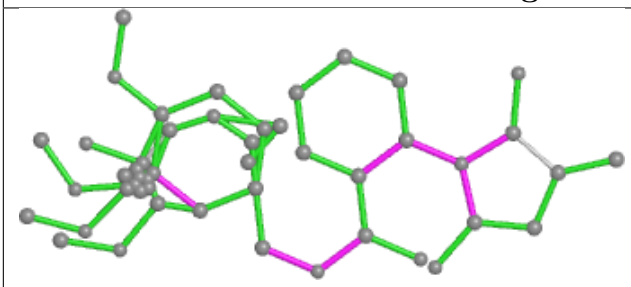
There are no ring outliers.

10 monomers are involved in 45 short contacts:

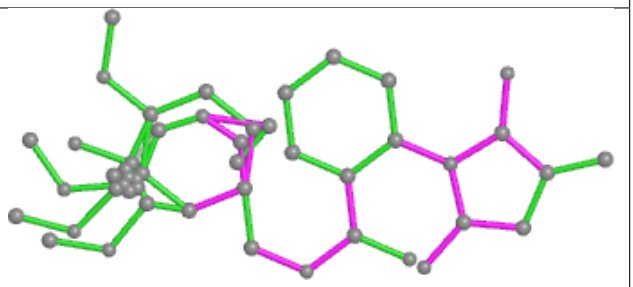
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	MLK	7	0
2	C	301	MLK	3	0
2	B	301	MLK	3	0
2	D	301	MLK	3	0
2	A	301	MLK	4	0
2	G	301	MLK	4	0
2	H	301	MLK	6	0
2	I	301	MLK	6	0
2	J	301	MLK	3	0
2	F	301	MLK	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

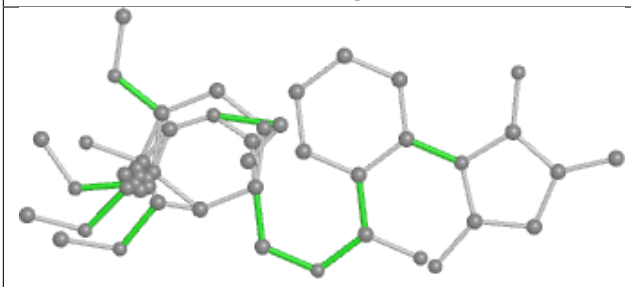
Ligand MLK E 301



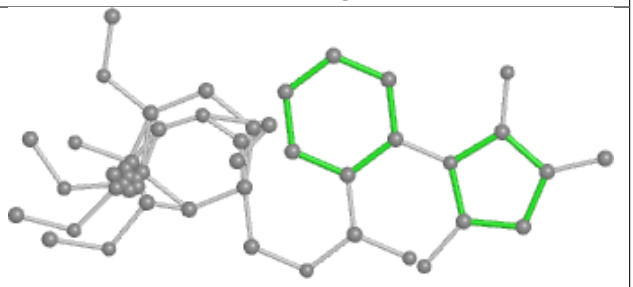
Bond lengths



Bond angles

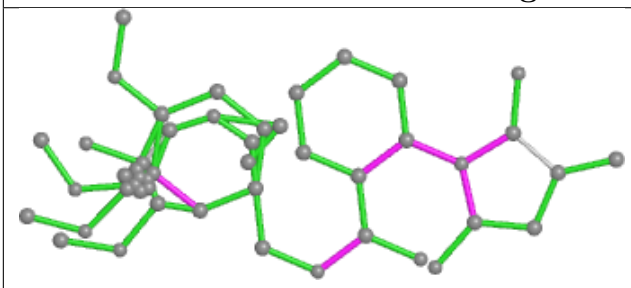


Torsions

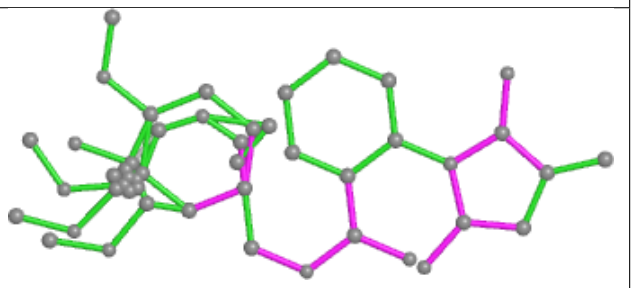


Rings

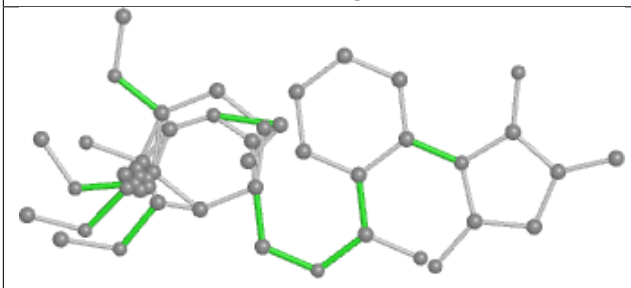
Ligand MLK C 301



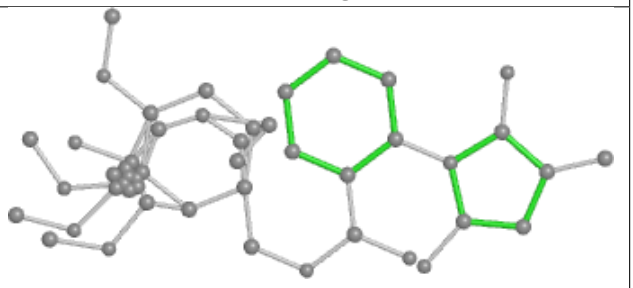
Bond lengths



Bond angles

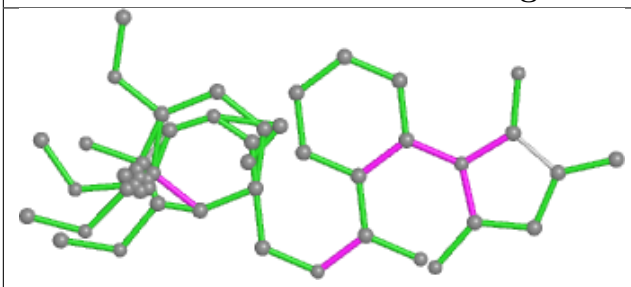


Torsions

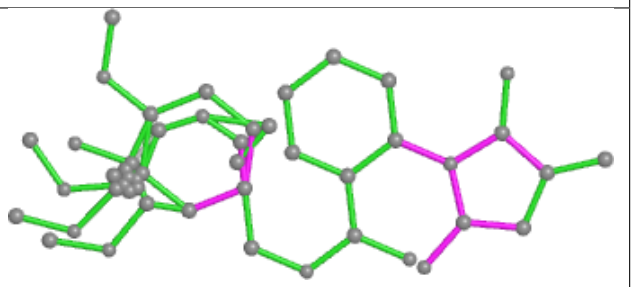


Rings

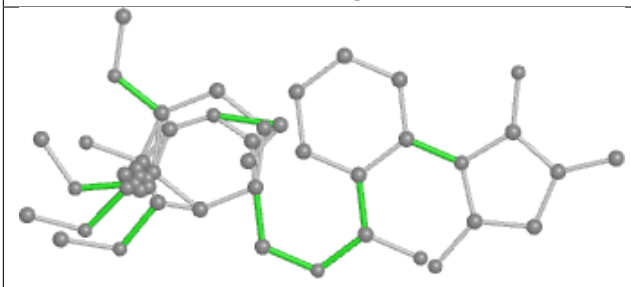
Ligand MLK B 301



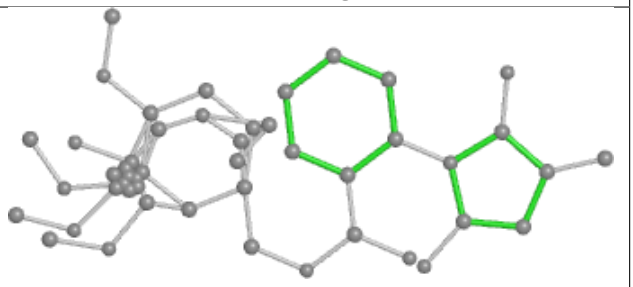
Bond lengths



Bond angles

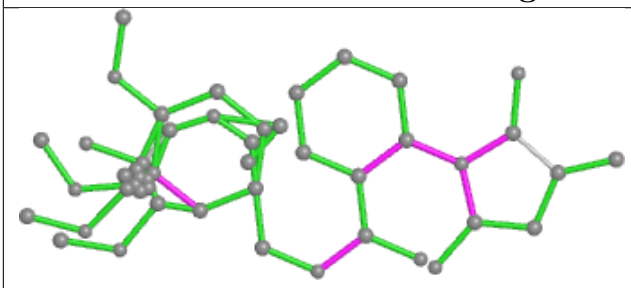


Torsions

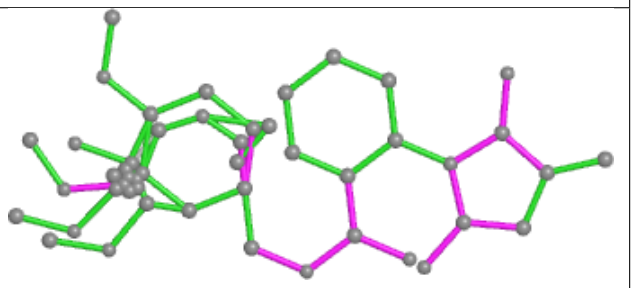


Rings

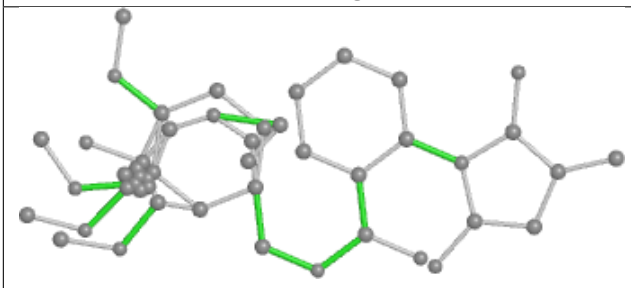
Ligand MLK D 301



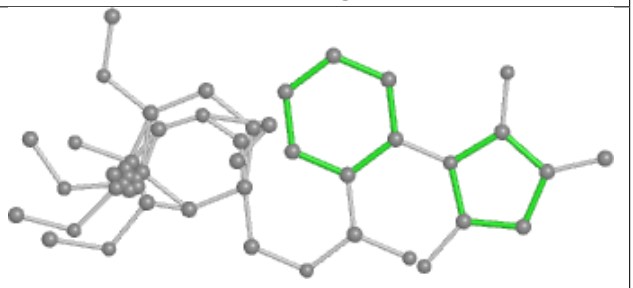
Bond lengths



Bond angles

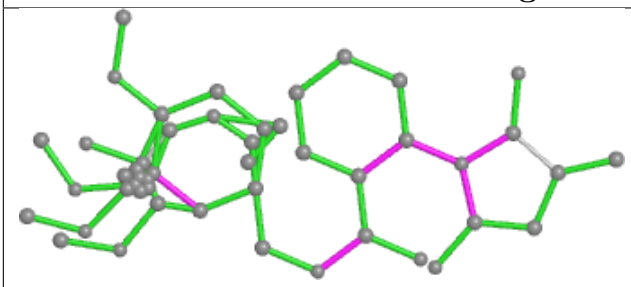


Torsions

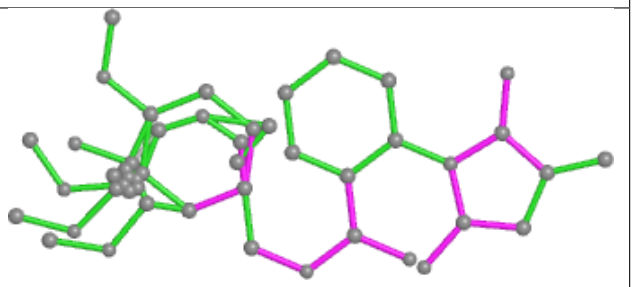


Rings

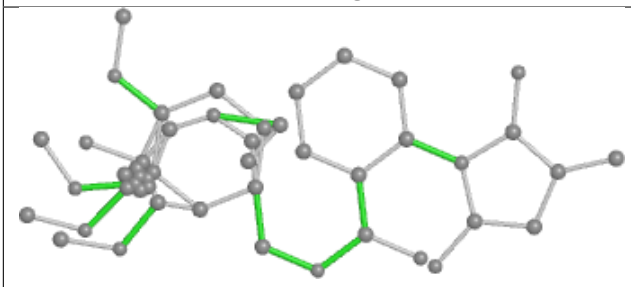
Ligand MLK A 301



Bond lengths



Bond angles



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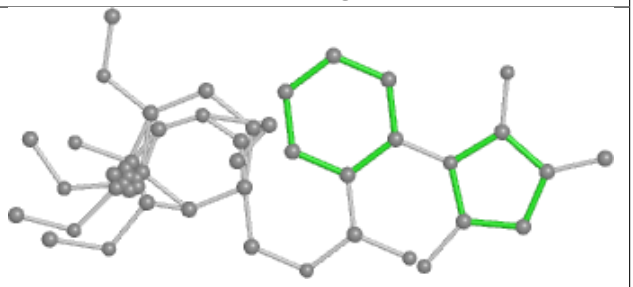
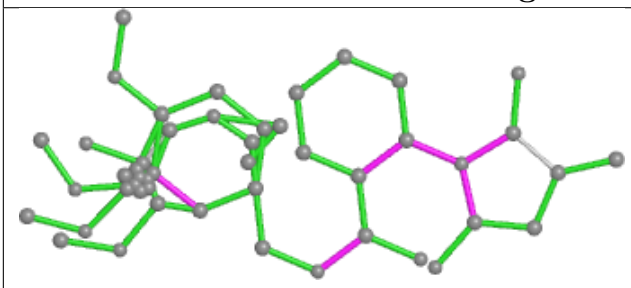
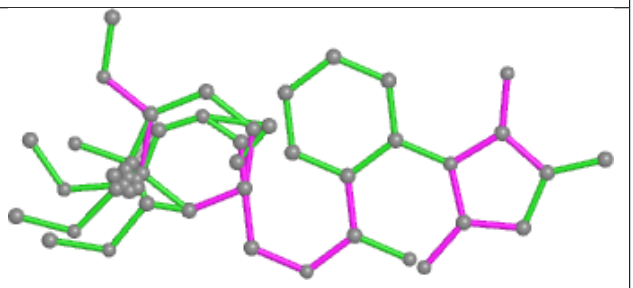


Rings

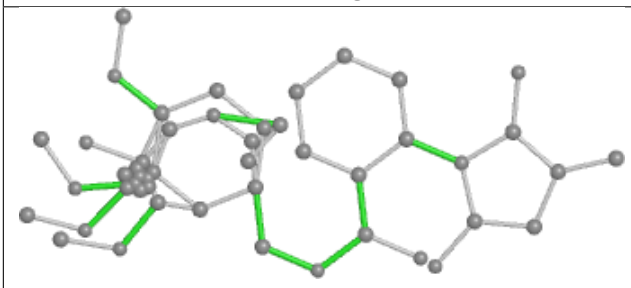
Ligand MLK G 301



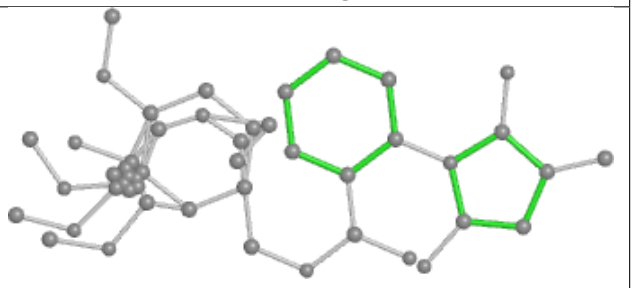
Bond lengths



Bond angles

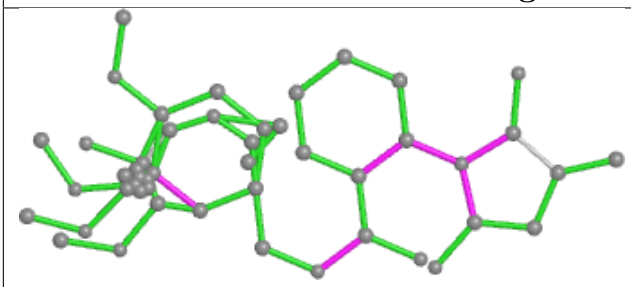


Torsions

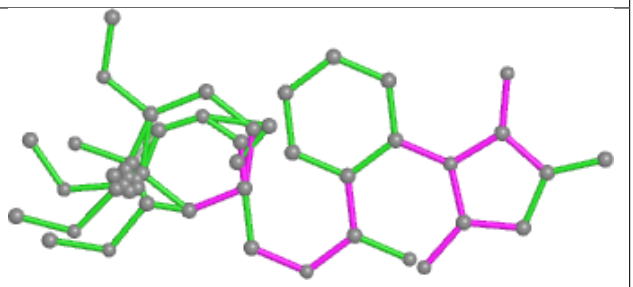


Rings

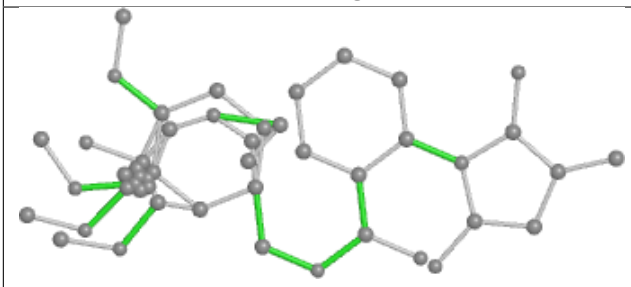
Ligand MLK H 301



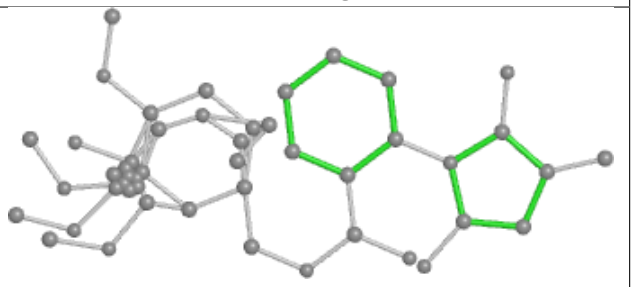
Bond lengths



Bond angles

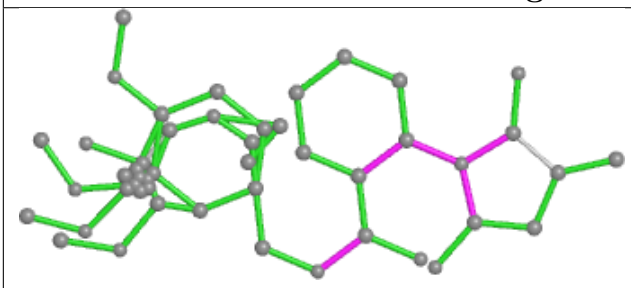


Torsions

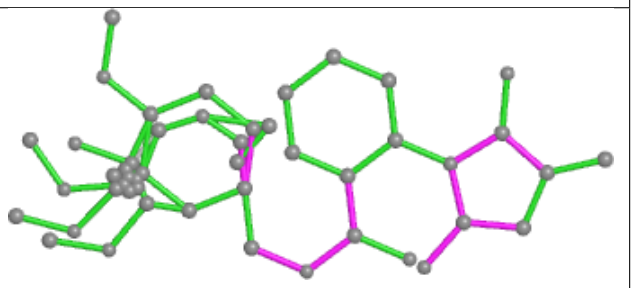


Rings

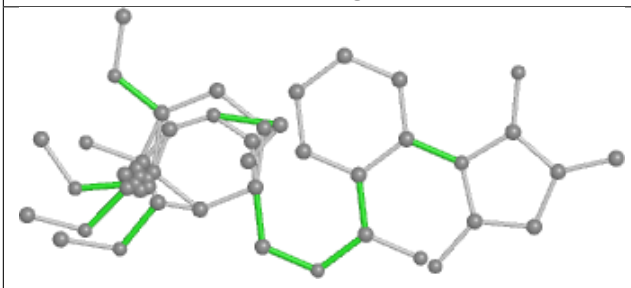
Ligand MLK I 301



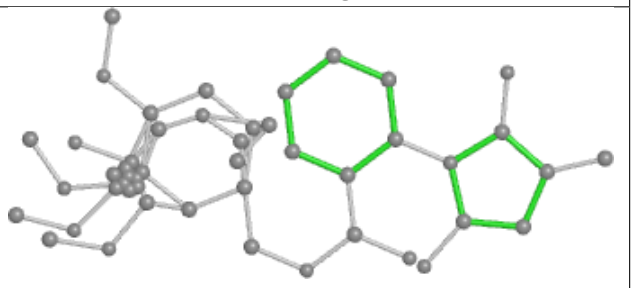
Bond lengths



Bond angles

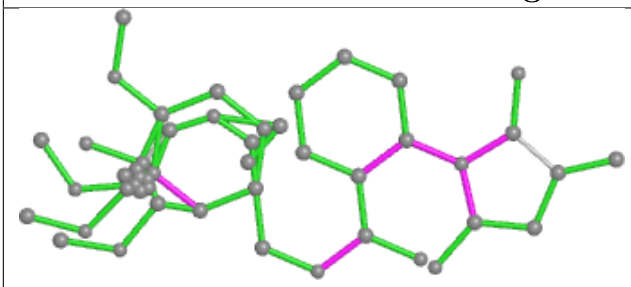


Torsions

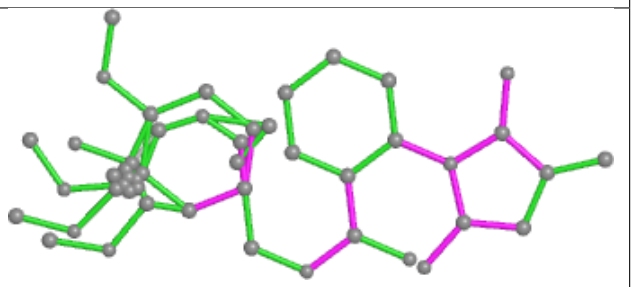


Rings

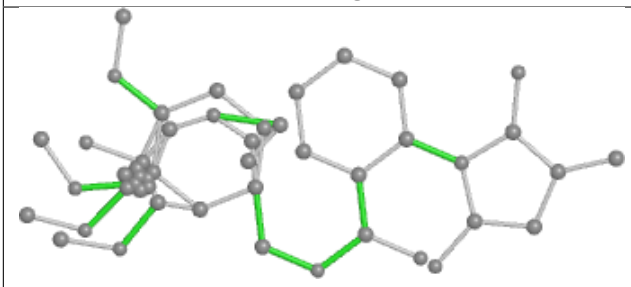
Ligand MLK J 301



Bond lengths



Bond angles



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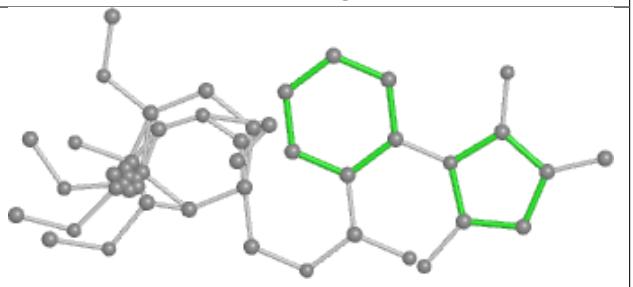
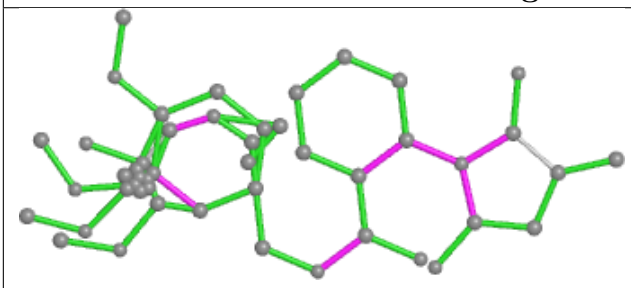
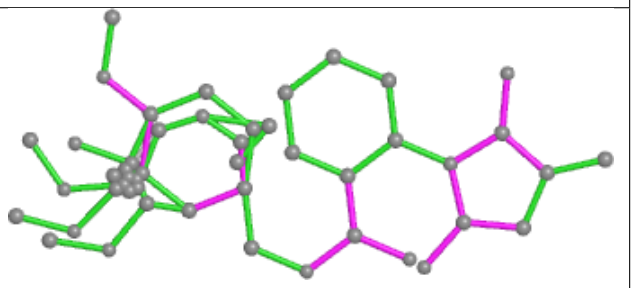


Rings

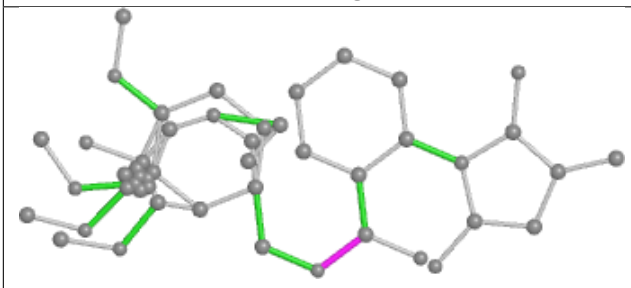
Ligand MLK F 301



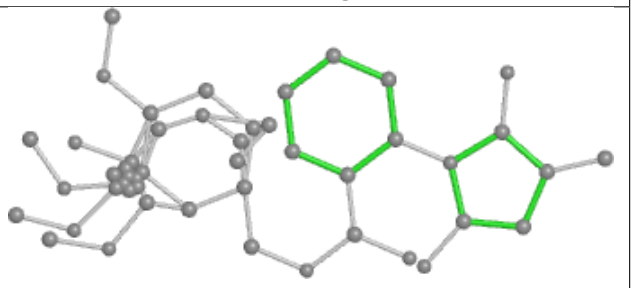
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	213/227 (93%)	0.10	3 (1%) 75 74	15, 28, 56, 77	0
1	B	210/227 (92%)	0.05	2 (0%) 82 83	14, 31, 62, 78	0
1	C	210/227 (92%)	0.05	4 (1%) 66 64	20, 38, 67, 96	0
1	D	211/227 (92%)	0.17	6 (2%) 53 49	22, 39, 74, 85	0
1	E	214/227 (94%)	0.06	3 (1%) 75 74	18, 30, 65, 92	0
1	F	209/227 (92%)	0.38	6 (2%) 51 47	29, 48, 75, 92	0
1	G	205/227 (90%)	0.36	6 (2%) 51 47	33, 55, 85, 95	0
1	H	204/227 (89%)	1.06	26 (12%) 3 2	45, 65, 95, 106	0
1	I	213/227 (93%)	0.38	10 (4%) 31 29	32, 51, 92, 100	0
1	J	212/227 (93%)	0.06	3 (1%) 75 74	22, 39, 69, 99	0
All	All	2101/2270 (92%)	0.27	69 (3%) 46 43	14, 43, 81, 106	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	ALA	5.4
1	H	16	ARG	5.2
1	I	190	CYS	5.0
1	H	1	HIS	4.6
1	H	33	LEU	4.4
1	F	19	MET	4.4
1	D	0	LEU	4.4
1	H	14	PHE	4.3
1	F	0	LEU	4.0
1	H	200	LEU	3.8
1	G	7	MET	3.6
1	D	19	MET	3.5
1	G	19	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	35	PHE	3.3
1	B	1	HIS	3.2
1	F	15	ASN	3.2
1	F	18	PRO	3.1
1	H	6	LEU	3.1
1	G	6	LEU	3.1
1	H	2	SER	3.0
1	H	15	ASN	3.0
1	E	-3	ASP	3.0
1	C	-2	ASP	2.9
1	C	0	LEU	2.9
1	C	208	ARG	2.8
1	E	16	ARG	2.8
1	D	17	SER	2.8
1	I	189	SER	2.8
1	H	156	LEU	2.7
1	I	18	PRO	2.7
1	H	74	ASN	2.7
1	H	65	LEU	2.7
1	J	1	HIS	2.7
1	G	18	PRO	2.7
1	H	125	PHE	2.7
1	H	71	GLU	2.6
1	D	15	ASN	2.6
1	H	70	ASN	2.6
1	H	157	LYS	2.6
1	H	154	ILE	2.5
1	A	0	LEU	2.5
1	I	22	GLY	2.5
1	J	38[A]	GLN	2.5
1	I	25	LYS	2.5
1	H	194	PRO	2.4
1	J	-3	ASP	2.3
1	I	0	LEU	2.3
1	I	1	HIS	2.3
1	E	18	PRO	2.3
1	F	16	ARG	2.3
1	G	13	LEU	2.3
1	C	16	ARG	2.3
1	A	17	SER	2.3
1	I	26	ASP	2.3
1	H	138	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	-4	ASP	2.2
1	H	37	LEU	2.2
1	H	108	VAL	2.2
1	D	16	ARG	2.2
1	H	152	PHE	2.2
1	D	18	PRO	2.2
1	H	20	TYR	2.1
1	H	135	GLU	2.1
1	F	75	ILE	2.1
1	H	57	GLN	2.1
1	H	201	VAL	2.0
1	I	15	ASN	2.0
1	I	17	SER	2.0
1	G	3	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MLK	I	301	49/49	0.88	0.21	49,52,56,57	0
2	MLK	H	301	49/49	0.89	0.17	51,52,59,59	0
2	MLK	G	301	49/49	0.90	0.18	45,46,56,56	0
2	MLK	A	301	49/49	0.93	0.14	28,30,40,40	0
2	MLK	D	301	49/49	0.93	0.17	39,40,45,45	0
2	MLK	F	301	49/49	0.93	0.18	43,44,48,48	0
2	MLK	C	301	49/49	0.95	0.14	30,32,40,40	0
2	MLK	E	301	49/49	0.95	0.16	27,28,37,38	0
2	MLK	J	301	49/49	0.95	0.15	30,33,39,39	0

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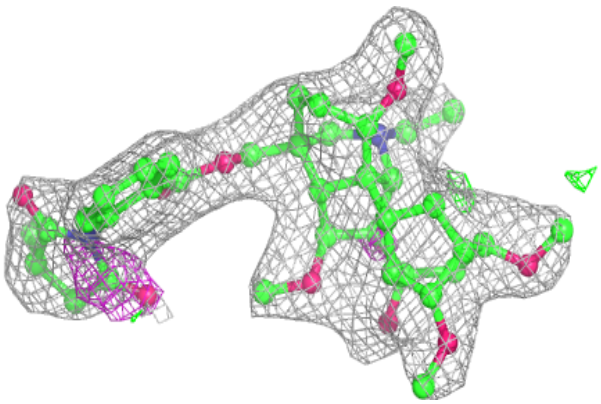
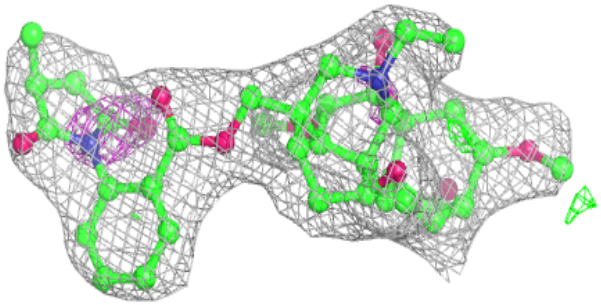
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MLK	B	301	49/49	0.96	0.14	23,25,31,32	0

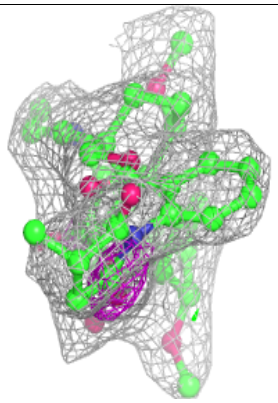
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MLK I 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

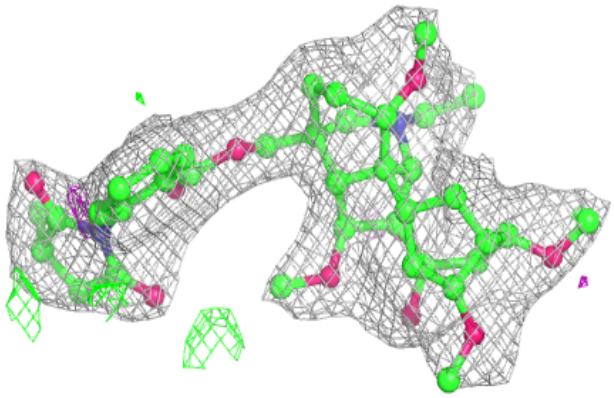


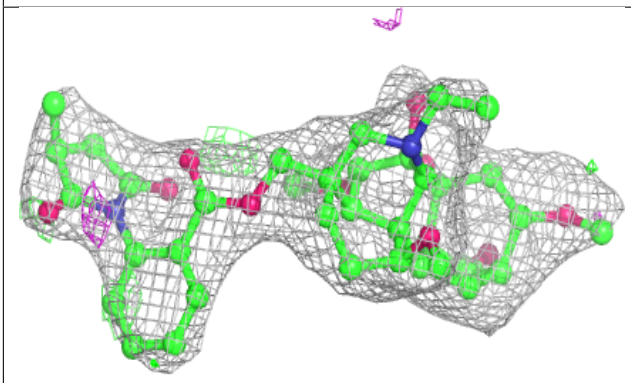


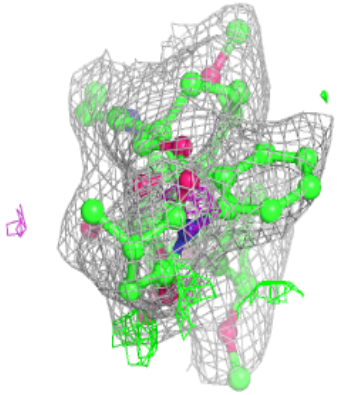


Electron density around MLK H 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

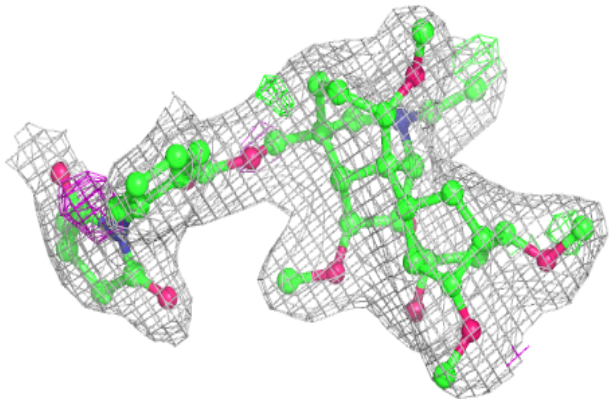


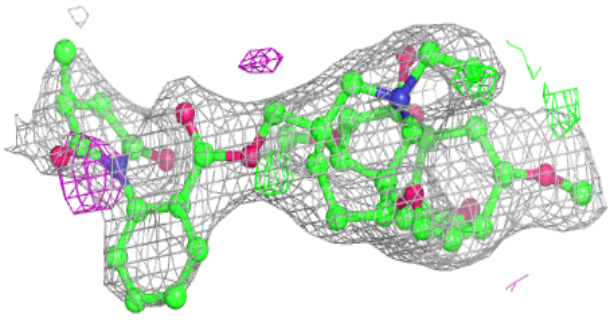


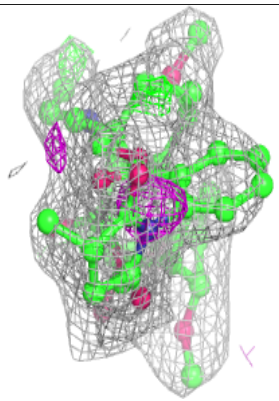


Electron density around MLK G 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

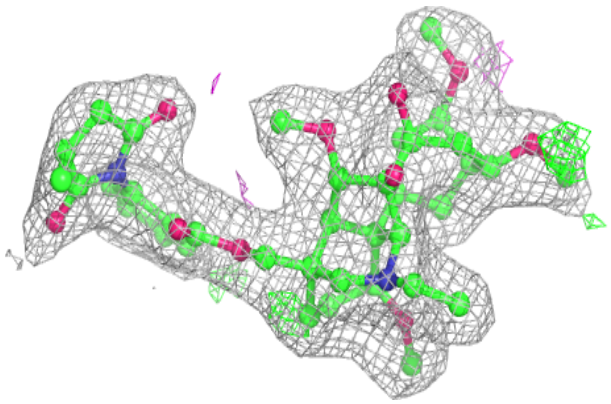


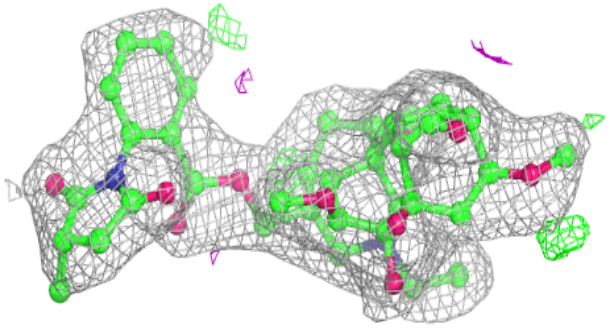




Electron density around MLK A 301:

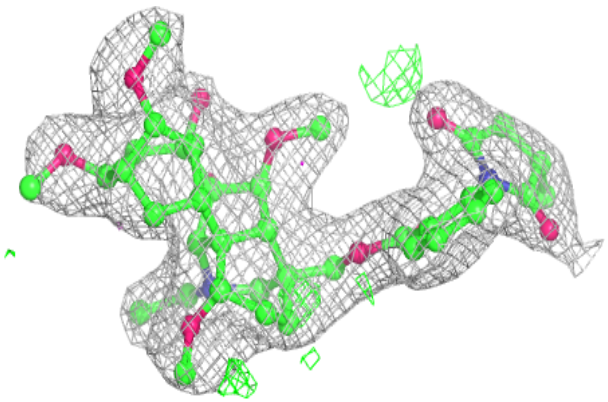
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

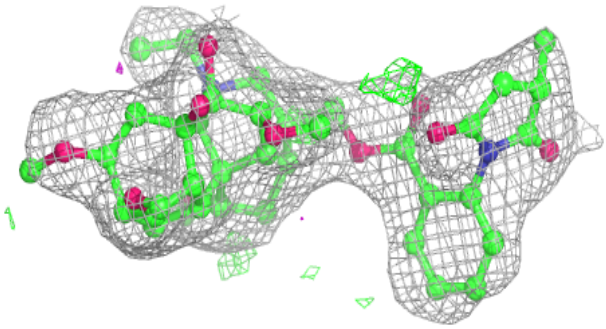


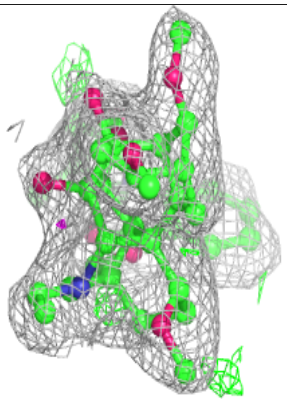


Electron density around MLK D 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

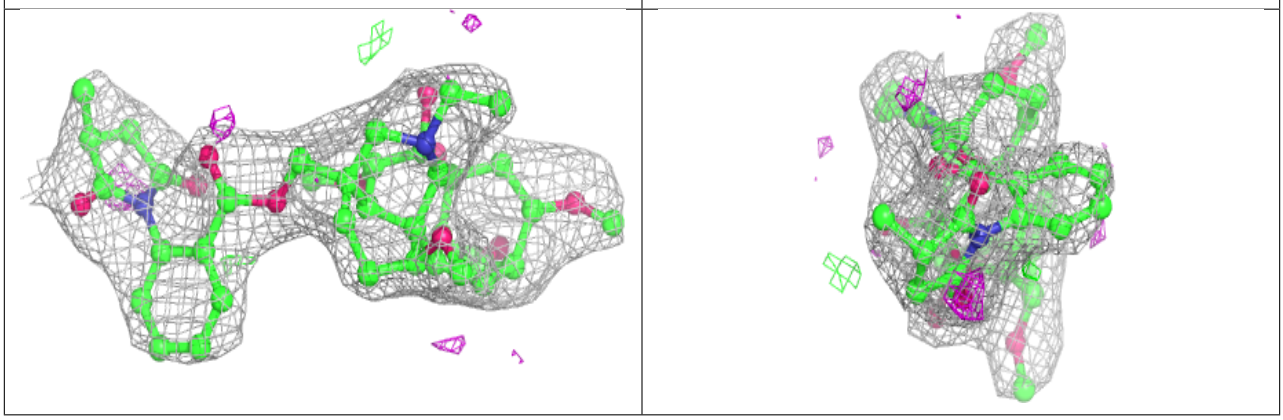






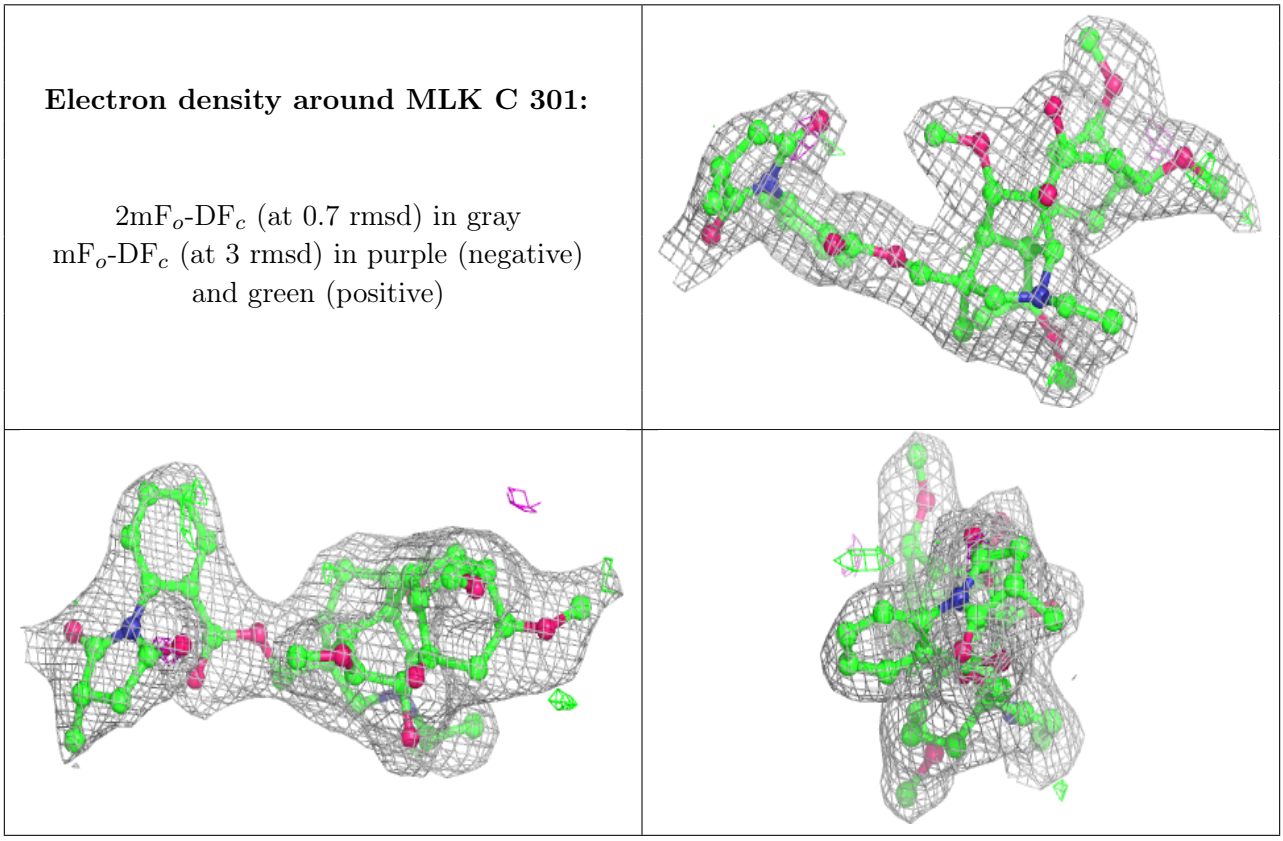
Electron density around MLK F 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



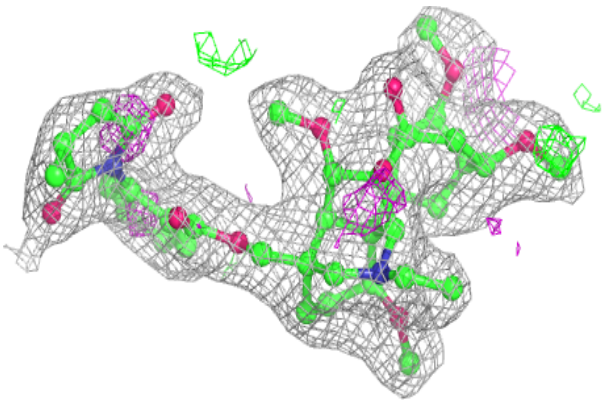
Electron density around MLK C 301:

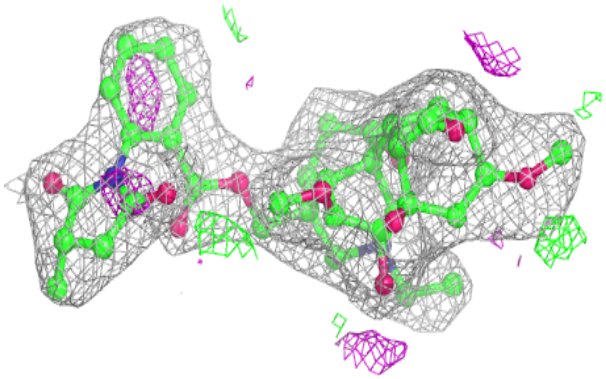
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

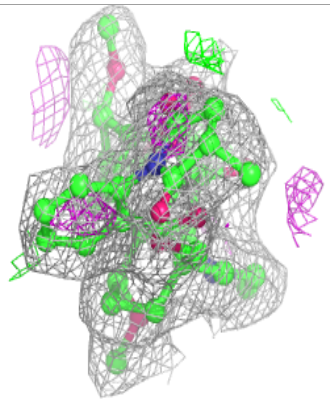


Electron density around MLK E 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

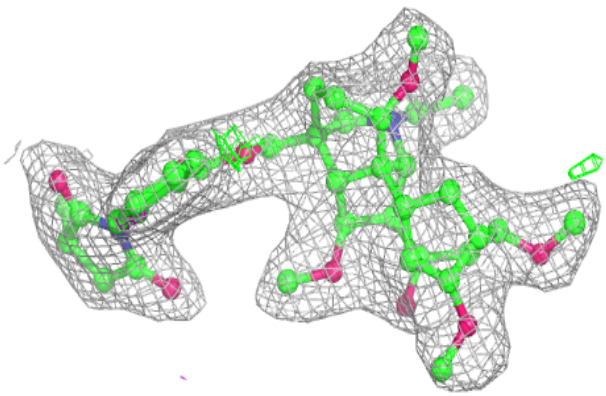


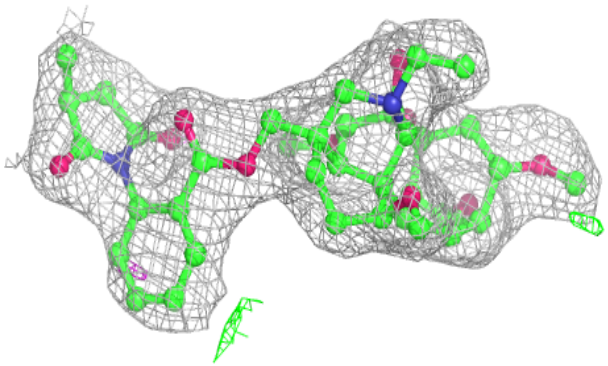


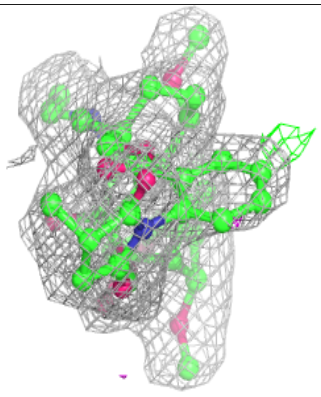


Electron density around MLK J 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

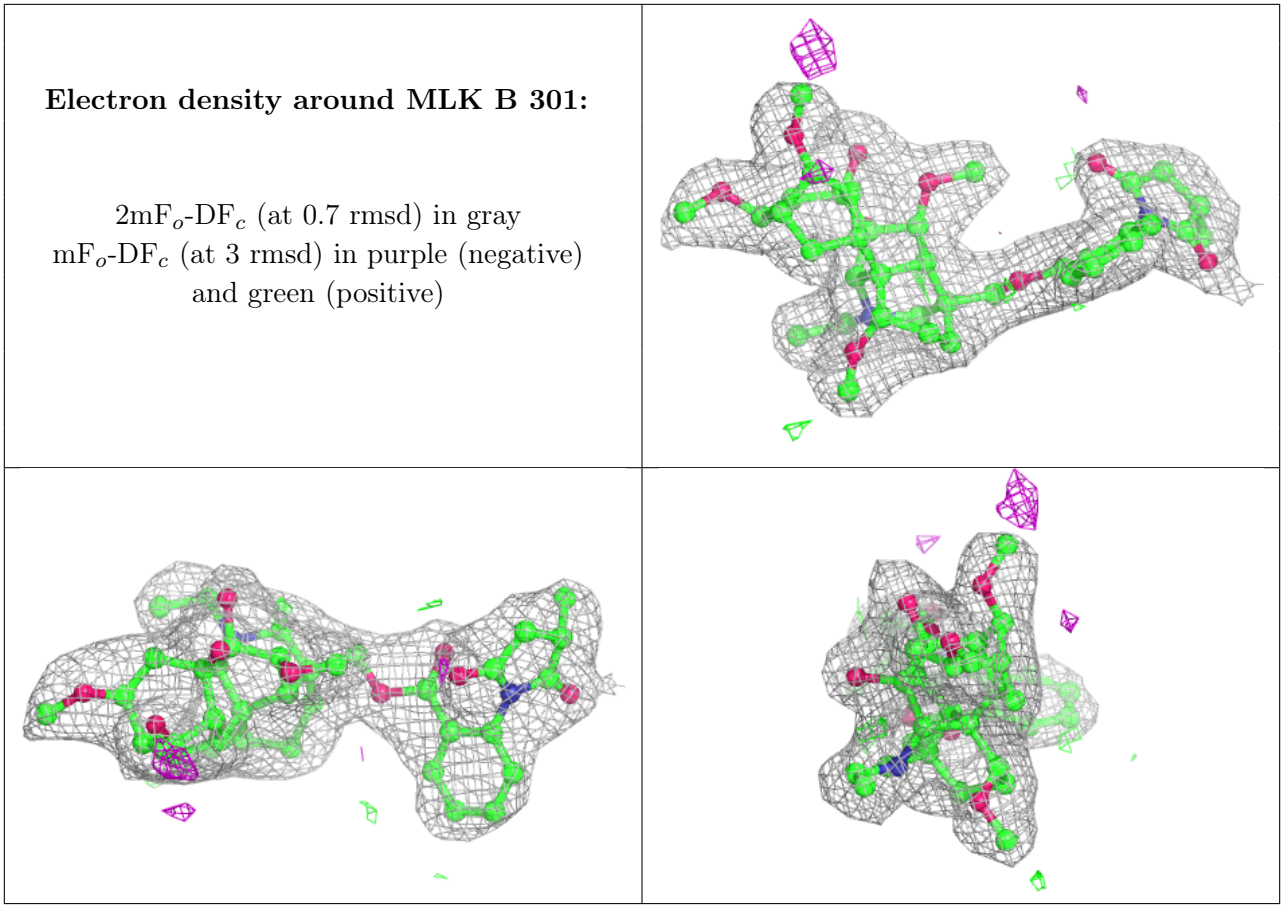






Electron density around MLK B 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.